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Green function for crystal surfaces I

Bernd Wenzien [1], Jörg Bormet, Matthias Scheffler

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin (Dahlem), Germany

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Abstract

The described computer code allows to calculate the surface Green function (SGF) of a semi-infinite solid with two-dimensional translational symmetry, using the layer Korringa–Kohn–Rostoker (KKR) approach within the muffin-tin approximation. The crystal is composed from planar or rumpled atomic layers, i.e., the atomic positions within the layer unit cell at the surface may differ from their ideal (bulk) values. The system may be divided into four regions of commensurable, two-dimensional lattice vectors, but with possibly different muffin-tin zeros and geometries: (i) vacuum region, (ii) overlayer, (iii) surface or subsurface region, (iv) substrate (bulk) region. The unit cell of any layer may be composed of any required number of different atoms. The Green function is evaluated in a spherical-wave expansion up to any maximum quantum number of angular momentum, with basis functions centered at the atomic sites. The following quantities can be computed from the SGF: (i) the electronic charge density, both for given energy E and Bloch vector $\boldsymbol{k}_{\parallel}$ and totally, i.e., integrated over E and $\boldsymbol{k}_{\parallel}$, and (ii) the local density of states (LDOS), either for a given $\boldsymbol{k}_{\parallel}$ and projected onto a given angular momentum, $L \equiv (l, m)$, (partial LDOS) or totally, i.e., integrated over $\boldsymbol{k}_{\parallel}$ and summed up over L.

PROGRAM SUMMARY

Title of program: fhi93g0

Catalogue number: ADAE

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Licensing provisions: Persons requesting the program must sign the standard CPC non-profit use license (see license agreement printed in every issue).

Computer, operating system, and installation:

- IBM RISC System/6000; AIX 3.2; FHI der Max-Planck-Gesellschaft, Berlin.
- CRAY Y-MP/4; UNICOS 7.0; IPP der Max-Planck-Geselschaft, Garching.
- CONVEX 220; ConvexOS (UNIX); FHI der Max-Planck-Gesellschaft, Berlin.
- Amdahl 370; UTS (UNIX System V); IPP der Max-Planck-Gesellschaft, Garching.
- SPECS TRITON; BSD UNIX; FHI der Max-Planck-Geselschaft, Berlin.

No. of bytes: 4288 Kbytes

Programming language used: FORTRAN 77, ANSI X3.9-1978 (exceptions from the standard are the use of `IMPLICIT NONE`, `DOUBLE COMPLEX`, and the C pre-processor `#include`-statement). The code is divided into four libraries.

Floating point arithmetic: 64 bits

[1] Present address: Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und Theoretische Optik, Max-Wien-Platz 1, D-07743 Jena, Germany.

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Memory required to execute with typical data: at least approximately 1.4 Mbytes, depending on machine and computational task

Remarks concerning installation of program
Programming is done in a rigorous modulare structure. All of the source files contain only one program unit (`PROGRAM`, `SUBROUTINE`, `FUNCTION`, `BLOCK DATA`) and are distributed over different subdirectories, corresponding to the different generated object module libraries and installations. A pre-processor has to be available for interpreting the C-like pre-processor statements within the source files during compilation. All the source files, including also shell scripts for compilation etc., may be extracted from the MS-DOS installation diskettes. For details, see the file `INSTALL`.

Keywords: Green function, surface, overlayer, charge density, density of states, layer KKR method, multiple scattering, solid state, condensed matter

References to other published versions of this program:
Cat. no.: AADF; *Title:* SURFACE GREEN'S FUNCTION; *Ref. in:* Comput. Phys. Commun. 38 (1985) 403;
Cat. no.: AAXZ; *Title:* SURFACE GREEN'S FUNCTION vers. 2; *Ref. in:* Comput. Phys. Commun. 47 (1987) 349;
Cat. no.: ABFF, *Title:* RUMPGF, *Ref. in:* Comput. Phys. Commun. 51 (1988) 381.
The first two papers are referred to below as paper or computer code I, the second paper is referred as paper or computer code II.

Nature of physical problem
The computer code (as that of papers I and II) allows to calculate the Green function (GF) for the one-electron Hamiltonian of a semi-infinite solid with two-dimensional translational symmetry parallel to the surface, within any given range of energy E. Thus, this surface Green function (SGF) satisfies the Bloch-type periodic boundary conditions parallel to the surface, for a given value of the Bloch vector $\boldsymbol{k}_{\parallel}$, and the boundary condition for outgoing waves normal to the surface. The following quantities describing the electronic structure may be computed from the SGF directly: (i) the electronic charge density within an arbitrary plane or box, both for given E and $\boldsymbol{k}_{\parallel}$ and totally, i.e., integrated over E and $\boldsymbol{k}_{\parallel}$, and (ii) the local density of states (LDOS), either for a given $\boldsymbol{k}_{\parallel}$ and projected onto a given angular momentum, $L \equiv (l, m)$, (partial LDOS) or totally, i.e., integrated over $\boldsymbol{k}_{\parallel}$ and summed up over L. In generalization to paper II, it is now possible to treat more complex systems with any number of different atoms composing the unit cell, e.g., reconstructed or rumpled clean surfaces as well as adsorbate systems.

Method of solution
The layer Korringa–Kohn–Rostoker (KKR) approach is used. The semi-infinite crystal is composed from layers parallel to the surface, and the atomic positions within the layer unit cell at the surface may differ from their ideal (bulk) values ("rumpled" layers). The potentials are treated within the muffin-tin approximation, and non-local pseudopotentials may be used. The system may be divided into four regions of commensurable, two-dimensional lattice vectors, but with possibly different muffin-tin zeros and geometries: (i) vacuum region, (ii) overlayer, (iii) surface or subsurface region, (iv) substrate (bulk) region. The unit cell of any layer may be composed of any required number of different atoms. The intra-layer scattering is treated by the method of Kambe [1], and the inter-layer scattering is treated using the layer-doubling scheme proposed by Pendry [2]. The Green function is evaluated using the method of Kambe and Scheffler [3] in a spherical-wave expansion up to any maximum quantum number of angular momentum, with basis functions centered at the atomic sites of the layers. Beginning with the top (overlayer or surface) region, the computational procedure is repeated layer-by-layer for the specified number of layers. The bulk Green function may be also evaluated.

Restrictions on the complexity of the problem
All substrate (bulk) layers are assumed to be identical, but, they may differ from the top layers (overlayer, surface, subsurface layers). The muffin-tin zero of the subsurface region has to equal that of the bulk region. If the Green function of the vacuum region is projected onto spherical waves, the number of centers for the expansion must not exceed the number of atomic sites per unit cell within the overlayer or top substrate layer, respectively. The two-dimensional lattice vectors of the different layers have to be commensurable to those of the corresponding (1×1) structure of the substrate.

Typical running time
The running time for the test run, i.e., one energy and $\boldsymbol{k}_{\parallel}$ point for a substitutional $(\sqrt{3} \times \sqrt{3})$ R 30° overlayer on the (111) surface of a fcc crystal, using 25 plane waves and 3 phase shifts per atom, and computing the Green function and LDOS for the overlayer, the first two subsurface layers, and the bulk, is:
- 20 s on IBM RISC System/6000, model 350,
- 4 s on CRAY Y-MP/4,
- 40 s on CONVEX 220,
- 60 s on Amdahl 370,
- 623 s on SPECS TRITON.

References
[1] K. Kambe, Z. Naturforschg. 22 a (1967) 322, 422; 23 a (1968) 1280.
[2] J.B. Pendry, Low Energy Electron Diffraction (Academic Press, London, 1974).
[3] K. Kambe and M. Scheffler, Surf. Sci. 89 (1979) 262.

LONG WRITE-UP

1. Introduction

The Green-function approach to the calculation of the electronic structure of crystals, introduced by Korringa [1], Kohn, and Rostoker [2], has enabled the ab initio, self-consistent determination of the atomic geometry and the electronic structure of perfect, three-dimensionally periodic crystals [3] within the density-functional formalism. In this paper, we describe a method to calculate the Green function for the single-electron Hamiltonian of a *semi-infinite* solid with two-dimensional translational symmetry parallel to the surface, using the layer Korringa–Kohn–Rostoker (KKR) approach within the muffin-tin approximation [4]. The most noticable feature of the surface Green function (SGF) formalism is the numerically accurate treatment of the problem despite the lack of translational symmetry perpendicular to the surface. Thus, the SGF approach is not restricted to finite clusters or slabs. Further, a minimal, chemically meaningful basis set may be used, i.e., all quantities characterizing the electronic structure, e.g., character of wave functions, electronic charge density, or local density of states (LDOS), may be given in terms of partial waves up to a finite quantum number of angular momentum, typically involving s, p, and d states, and are related directly to the SGF. The program described below is a generalization of the computer code of the papers I [5] and II [6] to more complex systems. The system may be divided into four regions of commensurable, two-dimensional lattice vectors, but with possibly different muffin-tin zeros and geometries: (i) vacuum region, (ii) top layer, e.g., adsorbate overlayer, (iii) surface or subsurface region, depending on whether an adsorbate overlayer is present or not, (iv) substrate (bulk) region. The unit cell of any layer may be composed of any required number of different atoms. For example, in the case of alkali adsorption on metals, considered here for the system Na/Al(111)-($\sqrt{3} \times \sqrt{3}$) R 30°, it is necessary to shift the muffin-tin potentials in the surface region upwards in energy, corresponding to an additional barrier between overlayer and substrate at fixed value of z parallel to the surface, for a proper description of the electronic structure. The reflexion and transmission properties of this additional step potential barrier are taken into account exactly. The spherical-wave expansion of the SGF within the vacuum region may be used for the projection of the SGF onto localized orbitals, as for example Gaussians [7], prior to the computation of surface electronic structure by means of a self-consistent method [8].

In the following section we summarize the method. The new computer code is described in Section 3, followed by a brief description how the programs could be installed (Section 4). The information about input data is given in Section 5, and the results of test runs are presented in Section 6.

2. The layer KKR Green function

The evaluation of the layer- and $\boldsymbol{k}_{\parallel}$-resolved KKR SGF proceeds in the same way as published in the papers I and II ($\boldsymbol{k}_{\parallel}$ is the two-dimensional Bloch vector). The semi-infinite system, described by muffin-tin potentials, is divided into possibly rumpled layers parallel to the surface, i.e., the atomic positions within the layer unit cell may differ from their ideal (bulk) values, and the layer KKR method of Kambe and Scheffler [4] is used. The computational scheme consists of two successive steps applied to each layer, beginning with the top layer, i.e., the overlayer or surface layer, respectively:

1. The layer of interest (labelled with λ) is left out, at first, and the Green function $G^{\lambda}_{\text{empty}}$, corresponding to the system where this layer is missing, is evaluated.
2. Then, the scattering at the layer omitted in the first step is included, and the complete Green function G^{λ}, valid in the region of the layer λ, is obtained.

Finally, this Green function $G^{\lambda}(\boldsymbol{r}' + \boldsymbol{R}', \boldsymbol{r} + \boldsymbol{R}; E, \boldsymbol{k}_{\parallel})$ of arguments $\boldsymbol{r}'$ and $\boldsymbol{r}$ within the muffin-tin spheres centered at the atomic sites $\boldsymbol{R}'$ and $\boldsymbol{R}$ is

given by the spherical-wave expansion

$$G^{\lambda}(\boldsymbol{r}'+\boldsymbol{R}', \boldsymbol{r}+\boldsymbol{R}; E, \boldsymbol{k}_{\parallel}) = \sum_{L'L} \Big[-\mathrm{i}\sqrt{2E}\, P^{\lambda}_{\boldsymbol{R}l}(E, r^{<}) \times H^{\lambda}_{\boldsymbol{R}l}(E, r^{>})\delta_{\boldsymbol{R}'\boldsymbol{R}}\delta_{L'L} + V^{\lambda}_{\boldsymbol{R}'L',\boldsymbol{R}L}(E, \boldsymbol{k}_{\parallel}) \times P^{\lambda}_{\boldsymbol{R}'l'}(E, r')\, P^{\lambda}_{\boldsymbol{R}l}(E, r)\Big] Y_{L'}(\hat{r}')\, Y_{L}^{*}(\hat{r}), \tag{1}$$

for each energy E, referring to the muffin-tin zero of the layer, and two-dimensional vector $\boldsymbol{k}_{\parallel}$. Here, $\delta_{\boldsymbol{R}'\boldsymbol{R}}$ and $\delta_{L'L}$ are Kronecker symbols, the $V^{\lambda}_{\boldsymbol{R}'L',\boldsymbol{R}L}$ describe the matrix of SGF coefficients, and the $P^{\lambda}_{\boldsymbol{R}l}$ and $H^{\lambda}_{\boldsymbol{R}l}$ are the solutions of the radial Schrödinger equation, corresponding to the following boundary conditions outside the muffin-tin sphere centered at site $\boldsymbol{R}$ of layer λ:

$$P^{\lambda}_{\boldsymbol{R}l}(E, r) = \tfrac{1}{2}\big[\mathrm{e}^{\mathrm{i}\delta_l} h_l^{(1)}(\sqrt{2E}\, r) + \mathrm{e}^{-\mathrm{i}\delta_l} h_l^{(2)}(\sqrt{2E}\, r)\big],$$

$$H^{\lambda}_{\boldsymbol{R}l}(E, r) = \mathrm{e}^{\mathrm{i}\delta_l} h_l^{(1)}(\sqrt{2E}\, r), \tag{2}$$

where $h^{(1)}$ and $h^{(2)}$ are the spherical Hankel functions of first and second order [9], $\delta_l \equiv \delta^{\lambda}_{\boldsymbol{R}l}(\sqrt{2E})$ are the scattering phase shifts of the atom at the site $\boldsymbol{R}$ within the unit cell of the layer λ, corresponding to the angular momentum l and the energy E. Further, the $Y_L(\hat{r})$ denote the spherical harmonics of the angular coordinates $\hat{r} \equiv (\theta, \phi)$ of the vector $\boldsymbol{r}$, corresponding to the angular momentum $L \equiv (l, m)$. Both the spherical Hankel functions and the spherical harmonics agree with the conventions given by Pendry [9]. The computational scheme uses the Ewald summation technique by Kambe [10] to treat the intra-layer scattering and the layer-doubling method proposed by Pendry [9] to treat the inter-layer scattering. Mathematical details are described in papers I and II.

The $\boldsymbol{k}_{\parallel}$-resolved and partial LDOS for any energy E, corresponding to atom $\boldsymbol{R}$ within the layer λ, may be obtained from the SGF via

$$N^{\lambda}_{\boldsymbol{R}L}(E, \boldsymbol{k}_{\parallel}) = -\frac{2}{\pi}\mathrm{Im}\int \mathrm{d}^3\boldsymbol{r}\, G^{\lambda}_{\boldsymbol{R}L,\boldsymbol{R}L}(\boldsymbol{r}, \boldsymbol{r}; E+\mathrm{i}0, \boldsymbol{k}_{\parallel}), \tag{3}$$

and the total LDOS is obtained by integrating the quantities $N^{\lambda}_{\boldsymbol{R}L}(E, \boldsymbol{k}_{\parallel})$ over the surface Brillouin zone (SBZ) and summing up over angular momentum L. The factor 2 in Eq. (3) takes the spin degeneracy into account. In the same manner, the spectral and partial charge density, reflecting the character of wave functions, is given by

$$n^{\lambda}_{\boldsymbol{R}L}(\boldsymbol{r}, E, \boldsymbol{k}_{\parallel}) = -\frac{2}{\pi}\mathrm{Im}\, G^{\lambda}_{\boldsymbol{R}L,\boldsymbol{R}L}(\boldsymbol{r}, \boldsymbol{r}; E+\mathrm{i}0, \boldsymbol{k}_{\parallel}). \tag{4}$$

Here, SBZ integration, L summation, and energy integration up to the Fermi level E_{F} yield the total charge density of valence electrons.

3. Program structure

The semi-infinite crystal can be composed of possibly rumpled atomic layers with commensurable two-dimensional lattice vectors parallel to the surface. The atoms of the two uppermost layers may differ from the atoms of the other (substrate) layers. The two-dimensional unit cell of any layer may consist of any required number of different atoms. With respect to the number of atoms per unit cell, maximum quantum number of angular momentum, number of plane waves, number of mesh points for the computation of charge density, etc., all the related array dimensions are calculated from the input data. The required storage for these arrays is allocated by the `SUBROUTINE ALCMAS`, and the data segment is splitted into the different array subsegments by the `SUBROUTINE LGDYNS`. In general, arrays passed to different program units are declared explicitely, but, auxiliary arrays are collected in the array `WS` which is used as work space to save computer memory. The only limit concerning the memory requirement of an actual calculation is given by the parameter `NDIMFO` in the include file `c_getmas.f`, determining the maximum amount of allocated storage, but this parameter may be increased if necessary.

In comparison with II the new code is fully reorganized. In general, numerical data are obtained by the program units via the parameter list

only. The usage of COMMON blocks is restricted to some control parameters. The declaration of such COMMON names is given by include files named c_*.f, thus, simplifying changes of them. BLOCK DATA sequences are contained in include files named b_*.f. The file c_lgprec.f contains limits of the machine accuracy used in different program units, assuming a 64 bit floating point arithmetic. Pre-definition of some parameters is done in the file c_lgparm.f.

The MAIN PROGRAM depends on the considered crystal structure and surface geometry, resulting in different surface Brillouin zones (SBZ). For example, the executable program lgfccsq3.x, treating the (111)-($\sqrt{3} \times \sqrt{3}$) R 30° surface of fcc crystals, is generated from the source file lgfccsq3.f, consisting of nothing but the appropriate include declarations for the include file f_lgprog.f, containing the PROGRAM LGPROG, the include file f_lgfccsq3.f, containing the corresponding SUBROUTINE LGRGET for the definition of lattice data, i.e., the irreducible part of the SBZ (ENTRY LGQSBZ), and the elements of point symmetry (ENTRY LGQSYM), and the include file f_gy2dhexa.f, containing the SUBROUTINE GYMESH generating the mesh for the integration over the irreducible part of the SBZ, i.e., here one sixth of a hexagon.

The program run is divided into the following steps which help to understand its logical structure:

Initial step

The input data defining computational task, dimensions, and control parameters are read by the SUBROUTINE LGDGET. The required storage is allocated by the SUBROUTINE ALCMAS, and the data segment is splitted into the different array subsegments by the SUBROUTINE LGDYNS which further calls the SUBROUTINE LGTASK to perform the computations.

Step 1

The required output files are opened by the SUBROUTINE LGDOOP, the input data concerning energy contours and $\boldsymbol{k}_{\parallel}$ points are read by the SUBROUTINE LGEGET and LGQGET, output to external files is written by the SUBROUTINE LGDOUT, LGEOUT, and LGQOUT. The pre-factors of the spherical harmonics and the Clebsch–Gordan coefficients are generated by the SUBROUTINE LGCELM. The geometrical and potential data are read by the SUBROUTINE LGVGET. If required, the mesh for the computation of electronic charge density is generated by the SUBROUTINE LGVGEN and LGMGEN and checked for several characteristics by the SUBROUTINE LGMCHK. Transformation of input data, e.g., concerning coordinate system, units of length, energy values, etc., is performed by the SUBROUTINE LGDTRA. The two-dimensional lattice vectors used in the Kambe summation [10] are generated by the SUBROUTINE LGRSET.

Step 2

The DO loop over the energy values taken as arguments of the SGF is performed. If required, the wave functions within the vacuum region are computed by the SUBROUTINE LGRWFO. The radial wave functions, scattering phase shifts, and radial integrals within the crystal region are obtained by the SUBROUTINE LGRWFB, calling the SUBROUTINE LGCPFI for their evaluation via the numerical solution of the radial Schrödinger equation by the predictor–corrector method [11] on a Herman–Skillman mesh [12]. These quantities may be written by the SUBROUTINE LGFOUT to an external file, allocated to unit ITMP(2), for usage in later runs, where they may be read by the SUBROUTINE LGFGET from unit ITMP(1).

Step 3

The DO loop over the $\boldsymbol{k}_{\parallel}$ points is performed for each energy. If the SGF is already computed and stored to an external file, the corresponding records of the input file, allocated to unit ITMP(1), are checked for completeness by SUBROUTINE LGGCOP, which copies the required records to a temporary file, allocated to unit ISI. Otherwise, the appropriate number of reciprocal lattice vectors $\boldsymbol{g}_{\parallel}$ (beams) used in the plane-wave representation is choosen by the INTEGER FUNCTION LGCALN, and their set is computed and factorized into Laue subsets by the SUBROUTINE LGQSET.

Step 4

This step will be skipped if the SGF already exists on an external file. Otherwise, the layer reflexion and transmission matrices are calculated for all individual layers by the SUBROUTINE LGMOTB, where the generation of the KKR structure constants [10] is performed by the SUBROUTINE LGMTKC.

Step 5

This step will be skipped if the SGF already exists on an external file. Otherwise, the reflectivity of the surface barrier and the propagators are calculated by the SUBROUTINE LGPROP. The mentioned surface barrier is assumed as a simple step function normal to the surface. The reflexion matrix of the semi-infinite substrate is computed by the SUBROUTINE LGBULK using the layer-doubling method [9] performed by the SUBROUTINE LGDBL.

Step 6

The DO loop over the layers in which the SGF matrix has to be evaluated is performed for each energy and $\boldsymbol{k}_{\parallel}$. If the SGF already exists on an external file, it is read by the SUBROUTINE LGGGET. Otherwise, the boundary-scattering matrices SL_j and SR_j (cf. Eqs. (8) and (9) of paper I) are calculated by the SUBROUTINE LGRSB.

Step 7

This step will be skipped if the SGF already exists on an external file. Otherwise, the empty-layer Green function G_{empty} is evaluated in a plane-wave representation and transformed to spherical waves centered at the atomic sites, calling the SUBROUTINE LGMSBB.

Step 8

The multiple scattering at the considered layer is evaluated, obtaining the coefficients $V^{\lambda}_{\bar{R}'L',RL}$

Table 1
Description of input and output units

Unit Specifier	Comment
IMI	Main input unit, connected to the standard input unit, i.e., IMI = 5, in dialog mode. Batch mode: IMI = 1, connected to the file SYSDTA.DAT (STATUS='OLD', ACCESS= 'SEQUENTIAL', FORM='FORMATTED') for default.
IMO	Main output unit, connected to the standard output unit, i.e., IMO = 6, in dialog mode. Batch mode: IMO = 2, connected to the file SYSLST.LST (STATUS='NEW', ACCESS= 'SEQUENTIAL', FORM='FORMATTED') for default.
ISI	Secondary input unit, used for the input of geometrical and potential data from an external file generated in a previous run, named GYLGPROG.VEC (STATUS='OLD', ACCESS ='SEQUENTIAL', FORM='FORMATTED') for default, and as I/O buffer for the SGF input, named GYLGPROG.TMP (STATUS='UNKNOWN', ACCESS= 'SEQUENTIAL', FORM= 'UNFORMATTED') for default. The filenames may be changed by input in dialog mode.
ISO	Secondary output unit, used for a secondary list file, named GYLGPROG.LST (STATUS ='UNKNOWN', ACCESS= 'SEQUENTIAL', FORM='FORMATTED') for default. The filename may be changed by input in dialog mode.
ITMP(1)	Temporary I/O unit, used for the input of wave functions and SGF from an external file generated in a previous run, named GYLGPROG.DAT (STATUS='OLD', ACCESS= 'SEQUENTIAL', FORM='UNFORMATTED') for default, or the output of geometrical and potential data to an external file required for a later run, named GYLGPROG.VEC (STATUS ='NEW', ACCESS='SEQUENTIAL', FORM='FORMATTED') for default. The filenames may be changed by input in dialog mode.
ITMP(2)	Temporary output unit, used for the output of wave functions and SGF to an external file required for a later run, named GYLGPROG.OUT (STATUS='NEW', ACCESS= 'SEQUENTIAL', FORM='UNFORMATTED') for default. The filename may be changed by input in dialog mode.
ITMP(3)	Temporary output unit, used for the output of electronic charge density to an external file, named GYLGPROG.RHO (STATUS='NEW', ACCESS='SEQUENTIAL', FORM ='FORMATTED') for default, and for the output of partial LDOS to external files, named GYLGxxxx.DAT (xxxx='0001', '0002', ..., STATUS='NEW', ACCESS ='SEQUENTIAL', FORM='FORMATTED') for default. The filenames may be changed by input in dialog mode.
ITMP(4)	Temporary output unit, used for the output of the radial mesh on which the charge density is evaluated. The external file is named GYLGPROG.CHK (STATUS='NEW', ACCESS ='SEQUENTIAL', FORM='FORMATTED') for default. The filename may be changed by input in dialog mode.

Table 2
Summary of executable programs

Program	Comment
lgbcc110.x	(110) surface, bcc lattice
lgfcc001.x	(001) surface, fcc lattice
lgfcc110.x	(110) surface, fcc lattice
lgfcc111.x	(111) surface, fcc lattice
lgfcc2x1.x	(001) surface, fcc lattice, (2 × 1) reconstruction
lgfccrow.x	(110) surface, fcc lattice, (1 × 2) reconstruction, e.g., missing row structure
lgfccsq2.x	(001) surface, fcc lattice, ($\sqrt{2} \times \sqrt{2}$) R 45° reconstruction
lgfccsq3.x	(111) surface, fcc lattice, ($\sqrt{3} \times \sqrt{3}$) R 30° reconstruction
lggra001.x	(0001) surface, graphite lattice
lgzns001.x	(001) surface, zinc-blende lattice
lgzns110.x	(110) surface, zinc-blende lattice
lgzns111.x	(111) surface, zinc-blende lattice
lgzns2x1.x	(001) surface, zinc-blende lattice, (2 × 1) reconstruction
lgpost.x	post-processor for output files containing electronic charge density

(cf. Eq. (1)) from the SUBROUTINE LGMSVC, if the spherical-wave expansion of the SGF is also required within the vacuum region, or by the SUBROUTINE LGMSLB, otherwise. If required, the SGF is written by the SUBROUTINE LGGOUT onto an external file, allocated to unit ITMP(2), for usage in later runs.

Step 9

The coefficients $V^{\lambda}_{\boldsymbol{R}'\boldsymbol{R},L'L}$ and the radial wave functions are combined to give the Green function $G^{\lambda}(\boldsymbol{r}'+\boldsymbol{R}', \boldsymbol{r}+\boldsymbol{R}; E, \boldsymbol{k}_{\parallel})$ for each energy E, Bloch vector $\boldsymbol{k}_{\parallel}$, and layer λ. This is performed by the SUBROUTINE LGRHO, obtaining the electronic charge density, and the SUBROUTINE LGLDOS, obtaining the, partial or local density of states (LDOS).

Final step

If required, the electronic charge density is written by the SUBROUTINE LGRTAB to an external file, allocated to unit ITMP(3), and the output of the LDOS is performed by the SUBROUTINE LGROUT.

The program may be run both in dialog or in batch mode. The description of the used input and output (I/O) units is given by Table 1. The set of these I/O units is divided into three subsets, i.e., (i) the main I/O units which are usually connected to the standard I/O units (in FORTRAN: units 5 and 6), (ii) the secondary I/O units which are connected to additional formatted I/O files, containing editable input data, e.g., describing the geometry and potentials, or de-

Table 3
The input data for the standard input unit

Format	Pattern	Comment
I1	MODE	= 0: Running the program in batch mode. Then, the further standard input is expected from the file SYSDTA.DAT, connected to unit IMI = 1, the main output is written to file SYSLST.LST, connected to unit IMO = 2 (cf. Table 1). This case is assumed, automatically, if the UNIX C shell script gylgprun without the _d flag or gylgpxgo (no flags) is used. = 1: Running the program in dialog mode. Then, the user is prompted for further input from the standard input unit (usually the terminal), the main output is written to the standard output unit (usually the terminal).

Table 4
The input data for unit IMI in batch mode

Format	Pattern	Comment
Secondary and temporary input and output units (cf. Table 1)		
6I5	ISI	Secondary unit for input.
	ISO	Secondary unit for output.
	ITMP	Temporary I/O unit(s).
Definition of computational task (cf. Table 5)		
10A8	DDOWRD	Keywords describing I/O operations.
10A8	TSKWRD	Keywords describing computational tasks.
10A8	LGFWRD	Keywords describing treatment of layer KKR SGF.
10A8	VECWRD	Keywords describing mesh generation for computation of charge density.
2A8	TYPE	CHARACTER*8 expression defining the lattice type.
	NSF	CHARACTER*8 expression defining the surface type. These expressions are checked by the corresponding program.
The following data record is only required if the keyword FILEIN is specified in DDOWRD, i.e., for the input of SGF from an external file generated in a previous run.		
2I5	NLO	Lower limit of layer index for which the SGF should be read from the external file, NLO $\geq$ 1.
	NLE	Upper limit of layer index for which the SGF should be read from the external file. NLE $\leq$ NL + 1 if the keyword BULK is specified in TSKWRD, i.e., for the additional computation of the bulk GF, otherwise NLE $\leq$ NL. The value of NL is specified in the previous run generating the external file (see below).
If the keyword FILEIN is specified in DDOWRD, the following data are read from the external files generated in a previous run. Then they have to be omitted in this main input file.		
A78		
A78	SCHR	CHARACTER*156 string containing comment. This comment is used to define the relation of output files for later runs.
3G10.0	DH	Miller indices of surface, corresponding to the coordinate system given by ASM1, ASM2, SURF (see below).
	DK	
	DL	
I5	NLT	Number of layer types. = 1: Substrate, only. = 2: The first layer is treated as overlayer, the second layer is treated as substrate. = 3: The first layer is treated as overlayer, the second layer is treated as substrate with the overlayer symmetry, and the third layer is treated as substrate with the bulk layer symmetry.
Dimensions of problem and control parameters		
If the keyword FILEIN is specified in DDOWRD, these data are read from the external files generated in a previous run. Then they have to be omitted in this main input file.		
The following data record is only required if the keyword VACUUM is specified in TSKWRD, i.e., for the spherical-ware expansion of SGF within the vacuum region.		
I5	NSUBO	Number of centers of SGF expansion within the (possibly rumpled) two-dimensional unit cell of the vacuum region.
3I5, G10.0	NRP(x)	Number of radial mesh points for the potentials of the layer x (upper limit).
	NB(x)	Number of different basis atoms within the layer x.
	NSUB(x)	Number of basis atoms within the (possibly rumpled) two-dimensional unit cell of layer x.
	EVPRDL(x)	Real part of the inner potential in eV, i.e., the muffin-tin zero of layer x with respect to the bulk muffin-tin zero.
The number of expected data records of the previous kind is given by NLT.		
5I5	NLPOT	Number of potentials per basis atom. = 1: One all-electron potential. > 1: For non-local pseudopotentials, NLPOT gives the number of different l-components. The potentials indicated by NLPOT are used for those values of l exceeding NLPOT, i.e., if $l \geq$ NLPOT.

Table 4 (continued)

Format	Pattern	Comment
	NBM	Number of beams used in the plane-wave representation of matrices (upper limit).
	NRM	Number of two-dimensional lattice vectors used by the Kambe summation in the elements of DLM2 (upper limit).
	ISPL	Number of intermediate points between radial mesh points on which the potential is given. This parameter is used for the integration of the radial Schrödinger equation in the SUBROUTINE LGCPFI by the predictor–corrector method and is typically set to 16.
	ISTEP	Number of radial Herman–Skillman mesh points with the same spacing, used for the integration of the radial Schrödinger equation. ISTEP is an input parameter of the SUBROUTINE LGCPFI, too, corresponds to the radial mesh of the potentials, and is typically set to 10.
6I5	LMAX	Maximum quantum number of angular momentum in the spherical-wave expansion.
	NL	Number of layers for which the Green function should be calculated.
	LFIX	Maximum number of layers used in layer doubling for computation of bulk reflexion and transmission matrices by SUBROUTINE LGBULK.
	NE	Number of energy points (totally, including all sections of the energy contour). This value is needed to allocate memory and will be recomputed by the program.
	NEC	Number of sections in the energy contour.
	NQP	Number of $k_{\parallel}$ points. This value will be recomputed by the program if the keyword SBZ is specified in TSKWRD, i.e., for the generation of $k_{\parallel}$ points within the irreducible part of the surface Brillouin zone.
5G10.0	GMAX	Maximum length of beams (in units of $2\pi/$SPA).
	DISO	Distance (in units of SPA) of the top crystal layer from the surface barrier.
	SPA	Unit of length in real space (in bohr). It must be equal to the (bulk) lattice constant if the keyword SBZ is specified in TSKWRD.
	EVPR	Real part of the inner potential in the bulk with respect to the vacuum level in eV.
	EVPI	Imaginary part of the inner potential added to all energy values along the energy contour. The total imaginary part of the energy values has to be positive to obtain convergency.
Dimensions and control parameters concerning special tasks		
The following two data records are only required if the keyword RHO is specified in TSKWRD, i.e., for the computation of the electronic charge density.		
5I5	NCM	Maximum number of atoms giving the centers for the SGF expansion ("cluster") which may contribute to the electronic charge density within the required box or planar layer. This value is needed to allocate memory.
	NPM	Maximum number of planar layers along which the electronic charge density should be evaluated. This value is needed to allocate memory.
	NX	Number of mesh points of the box or planar layer in x direction.
	NY	Number of mesh points of the box or planar layer in y direction.
	NZ	Number of mesh points of the box or planar layer in z direction.
G10.0	RMAX	Maximum length of two-dimensional translational vectors (in units of SPA) involved into the generation of "cluster" atoms for the computation of the electronic charge density.
The following two data records are only required if the keyword LDOS is specified in TSKWRD, i.e., for the computation of the local density of states.		
I5	NDEC	Number of steps in the analytical deconvolution of the LDOS back to the real energy axis. This is ingenious for the computation of the LDOS along the real axis within the complex energy plane, only. The deconvolution may be suppressed by setting NDEC = 0.
The following data record is only required if NDEC > 0 is specified.		
G10.0	ZIMD	Imaginary part of energy argument of the LDOS after the analytical deconvolution back to the real energy axis. The following condition should be valid: ESTEP = | 2*(ZIMO-ZIMD) / NDEC |, where ESTEP is the step width of the real part of energy, ZIMO is the imaginary part of energy before deconvolution.
The following data record is only required if the keyword LDOS is specified in TSKWRD, i.e., for the computation of the local density of states.		
I5	NPART	Number of start and end indices of angular momentum for the partial LDOS (see below).

Table 4 (continued)

Format	Pattern	Comment
Energy contour and $k_{\parallel}$ points		
If the keyword FILEIN is specified in DDOWRD, these data are read from an external file generated in a previous run. Then they have to be omitted in this main input file.		
2I5,	ILOOP(1)	Number of energy points in this segment of the energy contour (has to be odd).
4G10.0		
	ILOOP(2)	Kind of energy contour segment. = 1: The energy contour segment is a line. = 2: The energy contour segment is a rectangular box. Thus, two additional records of the same kind are expected. = 3: The energy contour segment is a semicircle.
	EC(1)	Real part of lower limit of energy contour segment in eV.
	EC(2)	Imaginary part of lower limit of energy contour segment in eV.
	EC(3)	Real part of upper limit of energy contour segment in eV.
	EC(4)	Imaginary part of upper limit of energy contour segment in eV. In the case of a rectangular box the lower limit of the second and third contour segments must coincide with the upper limit of the preceeding contour segment.
The number of expected data records of the previous kind is given by NEC.		
If the keyword POINTS is specified in TSKWRD, i.e., for the input of single $k_{\parallel}$ points, the following data record is expected.		
xG10.0	QP(1,.)	
	QP(2,.)	Components of $k_{\parallel}$ modulo a reciprocal lattice vector (in units of $2\pi/$SPA). The number of expected $k_{\parallel}$ points is given by NQP.
If the keyword LINE is specified in TSKWRD, i.e., for the generation of $k_{\parallel}$ points along a line, the following data record is expected.		
4G10.0	QPO(1,1)	
	QPO(2,1)	Components of $k_{\parallel}$ modulo a reciprocal lattice vector (in units of $2\pi/$SPA) at the lower limit of the $k_{\parallel}$ line.
	QPO(1,2)	Components of $k_{\parallel}$ modulo a reciprocal lattice vector (in units of $2\pi/$SPA) at the upper limit of
	QPO(2,2)	the $k_{\parallel}$ line.
If the keyword SBZ is specified in TSKWRD, i.e., for the generation of $k_{\parallel}$ points within the irreducible part of the surface Brillouin zone, no data records concerning $k_{\parallel}$ generation are required.		
Geometrical and potential data		
If the keyword FILEIN is specified in DDOWRD, these data are read from an external file generated in a previous run. Then they have to be omitted in this main input file.		
3G10.0	RVECO(.,1)	also called ASM1.
3G10.0	RVECO(.,2)	also called ASM2.
3G10.0	RVECO(.,3)	also called SURF. These vectors form a right-handed three-dimensional (not necessary orthogonal) coordinate system, referred to the cartesian coordinates x, y, z. All geometrical data correspond to this system.
The following NSUBO+1 data records are only required if the keyword VACUUM is specified in TSKWRD, i.e., for the spherical-wave expansion of SGF within the vacuum region.		
3G10.0,I5	RBASVC	Atomic coordinates (in units of SPA) of centers for the SGF expansion within the (possibly rumpled) two-dimensional unit cell of the vacuum region, referred to the directions given by RVECO. The first site of expansion has to be O(0, 0, 0).
	IBASVC	Kind of atomic site. This value is reset to zero by the program.
...		
3G10.0,I5	RBASVC	also called DIS(0). This vector describes the displacement (in units of SPA) from the origin of the vacuum region to that of the top layer of the crystal, referred to the directions given by RVECO.
	IBASVC	Kind of atomic site. This value is reset to IBAS1(1) by the program.

Table 4 (continued)

Format	Pattern	Comment
The number of the following data sets, describing the layer geometries and atomic potentials, is given by NLT.		
3G10.0,I5	RBASx	Atomic coordinates (in units of SPA) within the (possibly rumpled) two-dimensional unit cell of the layer x, referred to the directions given by RVEC0. The first atomic site has to be O(0, 0, 0).
	IBASx	Kind of basis atom, i.e., the index pointing to the corresponding potential data of the considered layer x, $1 \leq$ IBASx $\leq$ NB(x).
The number of expected data records of the previous kind is given by the parameter NSUB(x) of the corresponding layer x.		
3G10.0	RVEC(.,1,x)	also called ARI1(x),
3G10.0	RVEC(.,2,x)	also called ARI2(x). These vectors form the two-dimensional unit cell of the layer x, referred to the directions given by RVEC0, and are assumed to be measured in units of SPA.
3G10.0	RVEC(.,3,x)	also called DIS(x). This vector describes the displacement (in units of SPA) from the origin of this layer to that of the next layer deeper into the crystal, referred to the directions given by RVEC0.
The number of the following data subsets, describing the atomic potentials of the considered layer x, is given by NB(x).		
A8	NAME	CHARACTER*8 expression describing the type of potential.
4I5	NPARMx(.,1)	also called NRFCx. Number of radial mesh points up to the equidistant part of the integration mesh.
	NPARMx(.,2)	also called NRMTx. Number of radial mesh points up to the muffin-tin radius.
	NPARMx(.,3)	also called NRWSx. Number of radial mesh points in the Herman– Skillman-type mesh of the potential, e.g., up to the Wigner–Seitz radius, NRWSx $\geq$ NRMTx + 2, NRWSx $\leq$ NRP(x).
	NPARMx(.,4)	also called ISHFx. = 0: The parameter VSHFx (see below) is ignored. = 1: The potential is shifted by the constant value VSHFx.
	RPARMx(.,3)	also called ZNx. Atomic number of the considered atom. This value is reset to zero by the 4G10.0 program if the keyword PSEUDO is specified in LGFWRD, i.e., for using non-local pseudopotentials.
	RPARMx(.,4)	also called RMTx. Muffin-tin radius of the considered potential in bohr.
	RPARMx(.,5)	also called WBASx. Wigner–Seitz radius of the considered atom in bohr.
	RPARMx(.,6)	also called VSHFx. Constant shift of the considered muffin-tin potential in hartree. This value is ignored if ISHFx = 0.
xG10.0	RPx	Distance of the radial mesh points where the muffin-tin potentials are given, referred to the center of SGF expansion, in bohr. The first point has to be the origin (zero), the last two points have to be situated beyond the muffin-tin radius RMTx. Each successive group of ISTEP points (e.g., RPx(i), i = 2,..., ISTEP + 1, etc.) has to be of equidistant spacing with an interval twice of that of the previous group. The interval doubling continues until the index value NRFCx, for i > NRFCx the spacing between successive points remains unchanged.
	VPx	Radial muffin-tin potential(s) corresponding to the considered grid point in hartree. The pure potential is expected if the keyword VTIMESR is specified in LGFWRD, usually used in conjunction with the keyword PSEUDO in LGFWRD, specifying input of non-local pseudopotentials. Otherwise, the potential times radius is expected. The number of data is given by NLPOT.
The number of expected data records of the previous kind is given by the parameter NRWSx of the corresponding potential in the considered layer x.		
Additional data concerning special tasks		
The following four data records are only required if the keyword RHO is specified in TSKWRD, i.e., for the computation of the electronic charge density.		
3G10.0	CH	Miller indices of the planar layer(s) where the electronic charge density has to be computed, referred to the coordinate system given by ASM1, ASM2, SURF (see above).
	CK	
	CL	

Table 4 (continued)

Format	Pattern	Comment
3G10.0	RLIM(.,1)	
3G10.0	RLIM(.,2)	
3G10.0	RLIM(.,3)	Limits of mesh points describing the box or plane for the computation of the electronic charge density, referred to the directions given by RVECO (in units of SPA). These three points have to define a planar layer indicated by CH, CK, CL.

The following data record is only required if the keyword BODYGEN is specified in VECWRD, i.e., for the computation of the electronic charge density within a box.

3G10.0	RLIM(.,4)	Additional point completing the considered box, together with the preceeding three points.

The following data records are only required if the keyword LDOS is specified in TSKWRD, i.e., for the computation of the local density of states, and if NPART>0.

A8,2I5	PTEXT	CHARACTER*8 expression describing subblocks of partial LDOS.
	IPDOS	Start and end indices for the partial LDOS in terms of angular-momentum index $L = 2l + m + 1$, $1 \le L \le$ NL2, NL2=(LMAX+1)*(LMAX+1).

The number of expected data records of the previous kind is given by NPART.

Additional data concerning output of LDOS

The following data sets, describing output operations of results, are only required if the keyword LDOS is specified in TSKWRD, i.e., for the computation of the local density of states. In this case, the number of these data sets is NLE-NLO+1. Each data set, consisting of an arbitrary number of records of the following kind, has to be closed with an empty record. Default operations, specified by the keywords PLOT, PUNCH, and TAB in DDOWRD, are performed if the corresponding data set consists only of an empty line.

A8,2I5, 4G10.0,I5	OUTWRD	Keyword describing the kind of output operation. =PLOT: Output of results to the secondary list file in pseudo-graphic form. =PUNCH: Formatted output of results to external files for plotting. =TAB: Tabular output of results to the secondary list file.
	NFO	Lower index for output of the partial LDOS in terms of angular-momentum index $L = 2l + m + 1$, NFO ≥ 1.
	NFE	Upper index for output of the partial LDOS in terms of angular-momentum index $L = 2l + m + 1$, NFE $\le$ NL2, NL2=(LMAX+1)*(LMAX+1).

The following two data are only used if the keywords PLOT or PUNCH are specified.

	RPARM(1)	also called XMIN. Lower limit of argument (here, the real part of energy in eV) considered by the output operation.
	RPARM(2)	also called XMAX. Upper limit of argument (here, the real part of energy in eV) considered by the output operation.

The following three data are only used if the keyword PLOT is specified.

	RPARM(3)	also called YMIN. Lower limit of function (here, the partial LDOS in 1/eV) considered by the output operation.
	RPARM(4)	also called YMAX. Upper limit of function (here, the partial LDOS in 1/eV) considered by the output operation.
	IPARM(1)	=0: Plotting in dotted-line mode. =1: Plotting in solid-line mode.

tailed output lists, respectively, and (iii) all the remaining I/O units, called temporary I/O units, which are connected to external and possibly scratch files during the run of the program.

4. Making the programs

The executable programs which can be generated from the described computer code are sum-

Table 5
Description of keywords defining computational task

Keyword	Comment
Keywords DDOWRD *describing I / O operations*	
STDIN	Data input from the main input unit, e.g., the file named SYSDTA.DAT. Set by default.
STDOUT	Data output to the main output unit, e.g., the file named SYSLST.LST. Set by default.
FILEIN	Data input from external files generated in a previous run, additionally.
FILEOUT	Data output to external files required for a later run, additionally.
PROTFILE	Creation of a secondary list file, additionally.
PRINTALL	The highest print level, corresponding to the value of IPRINT in the include file c_lgparm.f, is set. Otherwise the program runs in silent mode, i.e., the output to the main output unit is minimized.
PLOT	Output of results (LDOS) to the secondary list file in pseudo-graphic form.
PUNCH	Formatted output of results (LDOS) to external files for plotting.
TAB	Tabular output of results (LDOS) to the secondary list file.
Keywords TSKWRD *describing computational tasks*	
DUMMY	No actions after data input. Set by default.
RHO	Computation of electronic charge density or character of wave functions.
LDOS	Computation of $\boldsymbol{k}_{\parallel}$-resolved local density of states.
VACUUM	Spherical-wave expansion of SGF and computation of required quantities within the vacuum region, additionally.
BULK	Computation of the Green function and the other required quantities within the bulk, additionally.
INTEGRAL	Integration of required quantities over $\boldsymbol{k}_{\parallel}$ within the surface Brillouin zone. The keyword SBZ has to be specified, additionally.
POINTS	Input of single $\boldsymbol{k}_{\parallel}$ points.
LINE	Generation of $\boldsymbol{k}_{\parallel}$ points along a line.
SBZ	Generation of $\boldsymbol{k}_{\parallel}$ points within the irreducible part of the surface Brillouin zone, e.g., for integration of required quantities.
Keywords LGFWRD *describing treatment of layer KKR SGF*	
DUMMY	No actions after data input. Set by default.
LGFCOM	Computation of layer KKR SGF.
LGFGET	Input of layer KKR SGF from an external file generated in a previous run. The keyword FILEIN has to be specified in DDOWRD, additionally.
LGFTAB	Tabular output of layer KKR SGF to the secondary list file.
SINGLE	The inter-layer scattering is skipped between different layers, i.e., the Green function for a multi-layer system is computed, instead of that corresponding to a semi-infinite crystal.
ERRSKIP	Errors in reading the external input file containing wave functions and SGF, generated in a previous run, are ignored, and the SGF is computed for the remaining energy and $\boldsymbol{k}_{\parallel}$ values, i.e., the keyword LGFCOM is set by the program. This keyword is ingenious, only, if the keyword FILEIN is specified in DDOWRD.
VTIMESR	The pure potential is expected and multiplied by the values of the radial mesh, usually used in conjunction with the keyword PSEUDO. The Coulomb-like potentials are often given in the form potential times radius, to avoid difficulties with the singularity at zero radius. This keyword must not be specified in the latter case.
PSEUDO	Input of non-local pseudopotentials is expected. The atomic numbers are reset to zero, corresponding to the boundary conditions for the radial wave functions at zero radius.
Keywords VECWRD *describing mesh generation for computation of charge density*	
These keywords are ingenious, only, if the keyword RHO is specified in TSKWRD, i.e., for the computation of the electronic charge density.	
VECGEN	Generation of translational vectors involved into mesh generation. Set by default.
CLEAVE	The generated set of atoms ("cluster") giving the centers for the SGF expansion is divided into planar layers, corresponding to the given Miller indices. Set by default.
RMESHGEN	Generation of mesh points for the computation of the electronic charge density. Set by default.
RMESHCHK	The generated mesh points are checked for several characteristics.
BODYGEN	The mesh points are generated within a three-dimensional box, otherwise within a two-dimensional plane, only.

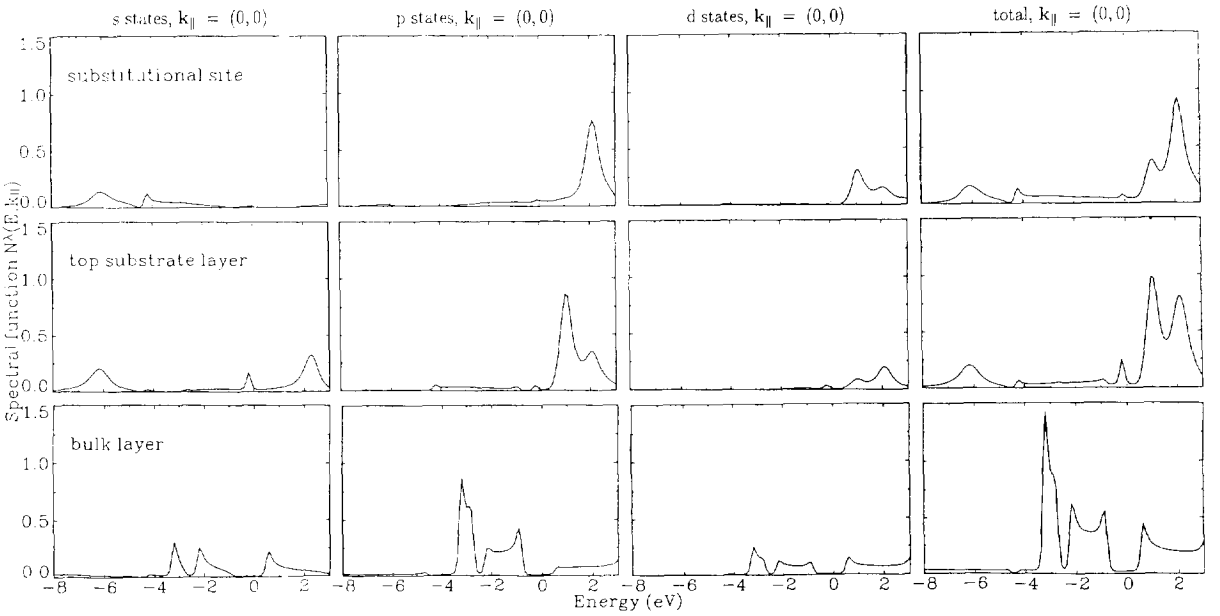

Fig. 1. Partial, $\boldsymbol{k}_{\parallel}$-resolved, and local density of states (spectral function), $N^{\lambda}(E, \boldsymbol{k}_{\parallel})$, for substitutionally adsorbed Na on the Al(111)-($\sqrt{3} \times \sqrt{3}$) R 30° surface at the $\bar{\Gamma}$ point of the SBZ, i.e., $\boldsymbol{k}_{\parallel} = (0, 0)$, and with λ labelling the adsorbate, top substrate, and the bulk layer. From the left to the right, the s, p, d contributions, and their sum are displayed. The energy is referred to the Fermi level, E_F, of bulk Al.

marized in Table 2. They should be made using the UNIX C shell scripts `install.bat`, `compile.bat`, and `link.bat`. These scripts and all the necessary source files are contained at the MS-DOS installation diskettes. Running the script `install.bat` will result in extracting the appropriate directory structure, containing the directories `nolim`, `mabif`, `clpr`, and `lgpr`, their subdirectories, the script and source files from these diskettes. Further, the source files are compiled and the object module libraries `nolim.a`, `mabif.a`, `clpr.a`, and `lgpr.a`, used to make the layer KKR programs, are generated by running the script `compile.bat`. Finally, the executable programs are made by running the script `link.bat`. A detailed description of installation is given in the file `INSTALL` contained at the diskette named `FOR_LGPR_1`. Additionally, the installation may be performed for UNIX systems from a compressed archive named `fhi93g0.tar.Z`, using the provided makefiles.

5. Input data

The input data for the standard input unit are described in Table 3. If the program is to run in batch mode, which is the usual way to use it, the flux of all possible input data read from the formatted input file `SYSDTA.DAT`, connected to unit `IMI = 1`, is given in Table 4. Though there is given a format specifier for each input pattern, data are read without any format, except the record contains `CHARACTER` names. The specification of the computational task including the physical problem to be considered is done by the keywords given in Table 5. Each of these keywords is of `CHARACTER*8` type and is to be padded with blanks only to the right.

6. Test runs

The input data of the test runs correspond to substitutionally adsorbed Na atoms on the

Al(111)-($\sqrt{3} \times \sqrt{3}$) R 30° surface [13]. We use non-local pseudopotentials [14], i.e., the muffin-tin potential $V^{\lambda}(\boldsymbol{r}+\boldsymbol{R})$ of argument $\boldsymbol{R}$ within the muffin-tin sphere centred at the atomic site $\boldsymbol{R}$ of the layer λ is given in a projection operator form,

$$V^{\lambda}(\boldsymbol{r}+\boldsymbol{R}) = \sum_{l=0}^{l=2} \sum_{m} V_{\boldsymbol{R}l}^{\lambda}(r)\ Y_{lm}^{*}(\hat{r}). \qquad (5)$$

The radial functions $V_{\boldsymbol{R}l}^{\lambda}(r)$ are obtained from self-consistent calculations [15] using the ab initio ionic pseudopotentials of Ref. [14]. The "overlayer" is built as a rumpled layer consisting of one Na atom, situated slightly above an empty Al site, and two Al atoms, the substrate layers consist of three equivalent Al atoms. For details concerning this structure and its physical properties we refer to Refs. [13,15]. The muffin-tin zero of the "overlayer" is choosen 3 eV above that of the substrate.

The results, i.e., the partial and $\boldsymbol{k}_{\parallel}$-resolved LDOS (cf. Eq. (3)) of the Na atom and the top Al atom are shown in Fig. 1 for the value $\boldsymbol{k}_{\parallel} = (0, 0)$, i.e., at the $\bar{\Gamma}$ point of the SBZ. For comparison, the LDOS of bulk Al is shown, too.

Acknowledgements

We thank F. Máca for helpfull discussions.

Note added in proof

The program fhi93g0 will be stored in the CPC Program Library as a compressed UNIX tar file. Therefore, the comments, in the Program Summary and in Section 4, on installation from MS-DOS diskettes are not relevant. Users should consult the README and INSTALL files contained in the tar file for the appropriate installation instructions.

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TEST RUN INPUT

File on UNIT IMI

```
    9   10   11   12   13   14                    ISI  , ISO  , ITMP
STDIN   STDOUT  FILEOUT PROTFILETAB
LDOS    BULK    POINTS
LGFCOM  VTIMESR PSEUDO

FCC     (SQ3-30)                                  TYPE , NSF
*** A L U M I N U M - AL(111)-(SQRT(3) X SQRT(3))-R 30 DEG *** GAMMA POINT ***
*** DR. B. WENZIEN, 05/06/92 *** DSN = test/test.xxx                      ***
   0.   0.   1.                                   DH   , DK   , DL
    2                                             NLT
  156    2    3   3.0                            NRP  , NB   , NSUB , EVPRDL
  134    1    3   0.                             NRP  , NB   , NSUB , EVPRDL
    3   25   37   16   10                        NLPOT, NBM  , NRM  , ISPL , ISTEP
    2    3 2048    1    1    1                   LMAX , NL   , LFIX , NE   , NEC  , NQP
  5.0       0.4184    7.515    11.3       0.     GMAX , DISO , SPA  , EVPR , EVPI
    0                                             NDEC
    3                                             NPART
    1    1   8.8       0.1       8.8       0.1  IE   , KIND , EMIN , EMAX
   0.            0.                             QP1  , QP2
   1.0           0.            0.               ASM1
   0.            1.0           0.               ASM2
   0.            0.            1.0              SURF
   0.            0.            0.            2  RBAS , IBAS        - 1-ST LAYER
   0.612372436   0.353553391   0.342         1  RBAS , IBAS
  -0.612372436  -0.353553391   0.342         1  RBAS , IBAS
   1.224744871   0.                           ARI1
   0.612372436   1.060660172   0.             ARI2
   0.204124145   0.353553391   0.9194         DIS
ALUMINUM                                      NAME
  121  121  134    0                          NRFC , NRMT , NRWS , ISHF
   3.0       2.65695   2.93683  0.            ZN   ,  RMT , WBAS , VSHF
  0.00000d+00  0.31540d+01 -0.97148d-01 -0.14379d+01
  0.22141d-01  0.31458d+01 -0.96908d-01 -0.14533d+01
  0.44283d-01  0.31384d+01 -0.96778d-01 -0.14667d+01
.....
  0.29448d+01  0.00000d+00  0.00000d+00  0.00000d+00
SODIUM                                                  NAME
  141  141  156    1                                   NRFC, NRMT, NRWS, ISHF
   1.00000   3.14400   3.47500   0.18464              ZN  ,  RMT,  RWS, VSHF
  0.00000D+00  0.10629D+01 -0.59828D-01 -0.32300D+00
  0.22457D-01  0.10580D+01 -0.64746D-01 -0.32799D+00
  0.44914D-01  0.10531D+01 -0.69421D-01 -0.33288D+00
.....
  0.34809D+01 -0.16125D+00 -0.16232D+00 -0.14471D+00
   0.            0.            0.            1  RBAS , IBAS        - 2-ND LAYER
   0.612372436   0.353553391   0.            1  RBAS , IBAS
  -0.612372436  -0.353553391   0.            1  RBAS , IBAS
   1.224744871   0.            0.               ARI1
   0.612372436   1.060660172   0.               ARI2
   0.204124145   0.353553391   0.577350269      DIS
ALUMINUM                                      NAME
  121  121  134    0                          NRFC , NRMT , NRWS , ISHF
    3.0       2.65695   2.93683  0.            ZN   ,  RMT , WBAS , VSHF
   0.00000d+00  0.31540d+01 -0.97148d-01 -0.14379d+01
   0.22141d-01  0.31458d+01 -0.96908d-01 -0.14533d+01
   0.44283d-01  0.31384d+01 -0.96778d-01 -0.14667d+01
```

```
.....................................................................................
  0.29448d+01  0.00000d+00  0.00000d+00  0.00000d+00
S           1    1
P           2    4
D           5    9
                                                                              EOR
                                                                              EOR
                                                                              EOR
                                                                              EOF
```

TEST RUN OUTPUT

File on UNIT IMO

```
.....................................................................................

 *** CONTROL     PRINT OF LATTICE DATA -

    FCC         LATTICE TYPE
    (SQ3-30)    SURFACE NORMAL DIRECTION

 *** CONTROL     PRINT OF TEXT -

 *** A L U M I N U M - AL(111)-(SQRT(3) X SQRT(3))-R 30 DEG *** GAMMA POINT ***
 *** DR. B. WENZIEN, 05/06/92 *** DSN = test/test.xxx                        ***

 *** CONTROL     PRINT OF MILLER INDICES OF SURFACE -

        DH    DK    DL
 ------------------------------------------------------------------------------
        0.    0.    1.

.....................................................................................

 *** DYNAMICAL SHARING OF STORAGE RESOURCES -

        48616 * 8 BYTES  REQUESTED
        48616 * 8 BYTES  AVAILABLE

 *** DYNAMICAL SHARING OF STORAGE RESOURCES -

           64 CHARACTERS REQUESTED
           64 CHARACTERS AVAILABLE

 *** CONTROL     PRINT OF PARAMETERS -

       NLT             NRP             NB            NSUB    NSUBVC
       NCM  NPM   NX   NY   NZ LMAX LPOT   NL  NLO  NLE LFIX  NBM  NRM   NE  NEC
       NQP NDEC PART ISPL STEP     ICELM NSMX LOX1  NL1  NL2 N2LM
           NRES      NWRK
 ------------------------------------------------------------------------------
         2  156  134    0    2    1    0    3    3    0         0
         0    0    0    0    0    2    3    3    1    4 2048   25   37    1    1
         1    0    4   16   10       126    3    3    3    9   15
         1    4      8875

.....................................................................................
```

```
*** CONTROL     PRINT OF ENERGY CONTOURS -

       I   IE KIND  RE(EMIN)  IM(EMIN)  RE(EMAX)  IM(EMAX)
-------------------------------------------------------------------------------
       1    1    1   8.80000    .10000   8.80000    .10000

    NE =   1   AFTER RECOMPUTATION
*** CONTROL     PRINT OF ENERGY VALUES -

       I     RE(E)     IM(E)     RE(E)     IM(E)     RE(E)     IM(E)
-------------------------------------------------------------------------------
       1   8.80000    .10000

*** CONTROL     PRINT OF PARALLEL WAVE VECTORS -

      I    QP1(I)    QP2(I)   I    QP1(I)    QP2(I)   I    QP1(I)    QP2(I)
-------------------------------------------------------------------------------
      1    .00000    .00000

*** CONTROL     PRINT OF BASIS VECTORS -

       I             X         Y         Z
-------------------------------------------------------------------------------
       1         1.00000    .00000    .00000
       2          .00000   1.00000    .00000
       3          .00000    .00000   1.00000

*** CONTROL     PRINT OF BASIS   ATOMS -

       I KIND         X         Y         Z
-------------------------------------------------------------------------------
       1    2    .00000    .00000    .00000
       2    1    .61237    .35355    .34200
       3    1   -.61237   -.35355    .34200

*** CONTROL     PRINT OF BASIS VECTORS -

       I             X         Y         Z
-------------------------------------------------------------------------------
       1         1.22474    .00000    .00000
       2          .61237   1.06066    .00000
       3          .20412    .35355    .91940

*** CONTROL     PRINT OF BASIS   ATOMS -

       I KIND         X         Y         Z
-------------------------------------------------------------------------------
       1    1    .00000    .00000    .00000
       2    1    .61237    .35355    .00000
       3    1   -.61237   -.35355    .00000

.....

*** END    OF   EXECUTION     IN PROGRAM /GYLGPROG/ -

    ELAPSED CPU TIME --- 00:00:19.84

*** TERMINATION BY SUBROUTINE /GYSTOP  / -

    CONDITION CODE IS   0 -

    NO SEVERE ERRORS DETECTED. EXITING.
```

File on UNIT ISO

```
 K-RESOLVED PARTIAL AND LOCAL DENSITY OF STATES OF SURFACE LAYERS
 ================================================================================

     LAYER  INDEX            ILT =          1
0    ENERGY INTERVAL FROM   EMIN =    8.80000   TO   EMAX =    8.80000
                         BY STEP =     .00000
0    PARALLEL WAVE VECTOR   QP1  =     .00000   ,    QP2  =     .00000
0    LAYER  INDEX    OF SUBLAYER =          1
 ------------------------------------------------------------------------------
OFCT NAME  IO         X(I)         X(I)         X(I)         X(I)         X(I)
 ------------------------------------------------------------------------------
           1   .88000D+01
 S       =     .65231D-02
 P       =     .51848D-01
 D       =     .11549D-01
 TOTAL   =     .69920D-01
 ------------------------------------------------------------------------------
0    LAYER  INDEX    OF SUBLAYER =          2
 ------------------------------------------------------------------------------
OFCT NAME  IO         X(I)         X(I)         X(I)         X(I)         X(I)
 ------------------------------------------------------------------------------
           1   .88000D+01
 S       =     .42305D-01
 P       =     .32963D-01
 D       =     .17180D-01
 TOTAL   =     .92448D-01
 ------------------------------------------------------------------------------
     LAYER  INDEX            ILT =          2
 ------------------------------------------------------------------------------
0    LAYER  INDEX    OF SUBLAYER =          1
 ------------------------------------------------------------------------------
OFCT NAME  IO         X(I)         X(I)         X(I)         X(I)         X(I)
 ------------------------------------------------------------------------------
           1   .88000D+01
 S       =     .18330D-01
 P       =     .40193D-01
 D       =     .23806D-01
 TOTAL   =     .82329D-01
 ------------------------------------------------------------------------------
 K-RESOLVED PARTIAL AND LOCAL DENSITY OF STATES OF BULK    LAYERS
 ------------------------------------------------------------------------------
OFCT NAME  IO         X(I)         X(I)         X(I)         X(I)         X(I)
 ------------------------------------------------------------------------------
           1   .88000D+01
 S       =     .13746D-01
 P       =     .22932D-01
 D       =     .14758D-01
 TOTAL   =     .51436D-01
 ------------------------------------------------------------------------------
```