



MSPHD: A full multiple scattering code for low energy photoelectron diffraction

R. Gunnella^{a,*}, F. Solal^b, D. Sébilleau^b, C.R. Natoli^c

^a *Unità INFN-Dipartimento di Mat. e Fisica, Università di Camerino, Via Madonna delle Carceri, 62032 Camerino (MC), Italy*

^b *Laboratoire PALMS, UMR CNRS-Université 6627, Université de Rennes, Campus de Beaulieu, 35042 Rennes, France*

^c *INFN, Laboratori Nazionali di Frascati, C.P. 13, 00044 Frascati, Italy*

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Abstract

We describe a Full Multiple Scattering (MS) code for the calculation of photoelectron diffraction (PD) patterns from solid surfaces. The use of a complex potential allows the calculation of complex phase shifts which describe realistically the damping of the electronic wave during its path to the detector. Full convergence in the scattering path expansion due to the inversion of the multiple scattering matrix makes this method particularly reliable in the surface sensitive energy range of the photoelectron, where approximate solutions in terms of series expansion and/or real potential calculations lead to inaccuracies in the determination of structural parameters. In this form the code is suitable to applications to clean surfaces such as Surface Core Level Shift Photoelectron Diffraction (SCLS-PD). © 2000 Elsevier Science B.V. All rights reserved.

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PROGRAM SUMMARY

Title of program: MSPHD

Catalogue identifier: ADMR

Program Summary URL: <http://cpc.cs.qub.ac.uk/summaries/ADMR>

Licensing provision: none

Computer: any

Operating system: open VMS, Unix

Program language: FORTRAN-77

Memory required: 1.5 mega words for the test case

No. of bits in a word: 64

No. of processors used: 1

Has the code been vectorised or parallelized?: No

No. of bytes of the source code: 369 316

No. of bytes in distributed program, including test data, etc.:
101 646

Distribution format: tar gzip file

* Corresponding author.

Keyword: Photoelectron Diffraction (PD), surface structure, surface, solid state, surface crystallography, multiple scattering, electron spectroscopy, reconstructed surfaces, core levels photoemission, surface core level shift

Nature of physical problem

Calculation of angle resolved and/or photon energy dependent photoemission from clean and adsorbed surfaces.

Method of solution

Implementation of the full multiple scattering theory with muffin-tin complex potential from self-consistent atomic charge densities to

the solution of the Schrödinger equation of a photoelectron detected in a particular direction by a high energy/angular resolution electron analyzer. The multiple scattering problem is solved by inversion of a symmetric complex matrix by means of the NAG Fortran package (subroutines F07QRF and F07QSF) and or by the equivalent LAPACK one (subroutines ZSPTRS and ZSPTRF).

Restrictions

Emission from s, p, d and f states only implemented.

Typical running time

For the test case 32 seconds on a DEC 4100 (400 MHz) EV56.

LONG WRITE-UP

1. Introduction

An efficient calculation method for full multiple scattering of the electron in photoemission is extremely useful in the assessment of surface potential effects on the shifted replicas of core level photoemission peaks [1]. Nevertheless the sensitivity of photoelectrons of such a low kinetic energy (about 50 eV), efficiently produced by a photoemission experiment at synchrotron radiation facilities, makes the PD technique suitable for probing structural properties of clean surfaces and adsorbate geometry [2]. The particular kinetic energy chosen is of strategic importance in the investigation of the influence of the interface with the vacuum in several topics such as in surface magnetism or in valence band photoemission. The present code, which has been used in obtaining the results of Ref. [1], and in other systems such as Si/Cu(110) and O/Ag(001) [3] is intended as a first step towards utilities capable of realistic descriptions of:

- (a) a general surface potential beyond the atomic muffin-tin approximation;
- (b) spin-dependent effects by inclusion of spin-orbit coupling in the final state;
- (c) correlation effects beyond the one-particle model by a multi-channel approach to the photoemission.

The present theory can be directly expanded to deal with these tasks. Finally the present code can perform photon energy scanned photoelectron diffraction by tuning the photoelectron energy. The latter experimental mode has been largely exploited as a quasi-direct method thanks to the properties of the back-scattering of electrons produced by molecules adsorbed on metals [4], and has many interesting applications such as a holographic method in photoemission by the phase-summing method [5]. In the low kinetic energy range where the multiple scattering acts as a quasi-random-phase generator which produce the necessary spherical wave-front for the holography the method could be even more efficient. It is in fact the non-spherical nature of the electronic wave which is the main limitation to the development of the photoelectron holography.

2. Theoretical framework

Very few codes are available to experimentalists with a user-friendly calculation interface for PD. A recent package has been proposed by Saldin and coworkers [6] by the concentric shell algorithm (CSA) which can be used over a large kinetic energy range. The present program is tailored to work at very low kinetic energy (30–100 eV) where it can optimize execution time and memory storage with respect to the CSA method. This will be even more effective as the physics increases in complexity as in the above cases (a), (b) and (c). Another

peculiarity of the present code is that it is self-contained with no inputs from other codes. The present program implements by a compact formalism the photoemission cross-section in a manner similar to the three-step-model, obtained by writing the multiple scattering final state photoelectron wavefunction in a piecewise potential (muffin-tin potential) [7]:

$$\frac{d\sigma}{d\hat{k}} = 8\pi^2 \alpha \omega \frac{k}{\pi} |S(\omega)|^2 \sum_{m_0} \left| \sum_j \sum_{LL'} M_L^{L_0} \tau_{LL'}^{oj, i'} Y_{L'}(\hat{k}) e^{i\vec{k} \cdot \vec{R}_{jo}} \right|^2. \quad (1)$$

Eq. (1) represents the value in Megabarns (Mb) of the angular photoemission cross-section along the direction $-\vec{k}$ (pointing to the electron analyzer) of a photoelectron originating at the atomic site “*o*” as a result of the absorption of a photon of energy ω . It propagates through the solid up to the atom “*j*” and then escapes into the vacuum. Quantities are expressed in Rydberg atomic units. The electron kinetic energy is k^2 , while α is the fine structure constant (1/137). The propagation of a spherical wave of angular momentum $L = (l, m)$ in the constant part of the potential outside the atomic sphere from the site “*i*” to the site “*j*” is described by Eq. (2):

$$G_{LL'}^{ij} = 4\pi \sum_{L''} i^{l+l''-l'} C_{LL'}^{L''} [-i h_{l''}^+(kR_{ij})] Y_{L''}(\hat{R}_{ij}) \quad (2)$$

which is written in terms of Hankel spherical waves $h_{l''}^+$ and Gaunt coefficients $C_{LL'}^{L''}$. The scattering events are taken into account by the atomic t -matrices

$$T_{L,L'}^{i,j} = t_i^i \delta_{ij} \delta_{ll'} = e^{i\delta_i^j} \sin \delta_i^j \quad (3)$$

with complex phase-shifts (δ_i^j), obtained by matching at the sphere radius the analytical solution outside the atomic sphere potential and the numerical solution inside the atomic spheres potential. In this way the multiple scattering problem can be solved to any order by the introduction of the scattering path operator

$$\tau_{LL'}^{ij} = [(T^{-1} + G)^{-1}]_{LL'}^{ij} \quad (4)$$

which includes all the scattering events of the electron in the solid. The factor $|S(\omega)|^2$ takes into account the oscillator strength associated with the completely relaxed channel of the final state. Eq. (1) is then easily interpreted in the three-step-model: (1) generation of an electron by the X-ray photon with matrix element $M_L^{L_0}$, the electric dipole operator matrix element between the initial state one-electron wavefunction (angular momentum L_0) and the final state of the continuum depending on the status of the polarization of the light. Then the electron propagates in the solid through the scattering path operator and is emitted in the vacuum as a plane wave in the $-\vec{k}$ direction. From the atomistic point of view no other ingredients must be added to the photoelectron diffraction formulation. By means of the built-in complex potential of the Hedin–Lundqvist type [8] the attenuation of the electronic wave during the scattering path is automatically taken into account. Finally the contribution from several absorbing atoms is incoherently added with relative weight given by the exponential decay of the electron wave from the absorbing atom to the surface. The code does not take into consideration the refraction rule at the surface potential barrier as it calculates photoemission for internal polar angles. The present approach shares with the CSA method the great advantage that the solution of the multiple scattering problem (the time expensive part of the whole task) can be performed by calculation of the operator of Eq. (4) once for each electron kinetic energy for the whole set of emission directions. Other methods which exploit the two-dimensional periodicity on the surface [9], or those which uses the multiple scattering expansion [10], depend on the emission direction and are expensive in time when a large set of angular data is collected on the whole hemisphere of emission from a surface (at least if a separable formalism [11] is not adopted). Finally the main drawback of multiple scattering series expansion methods is the bad convergence at very low kinetic energy.

3. Program structure of MSPHD

MSPHD calculates photoelectron diffraction patterns in 4 steps:

- (a) a cluster potential calculation (routine VGEN);
- (b) generation of a symmetrized basis functions to describe the final state wavefunction which transforms according to the representations of the point group of the surface (routine MOLSYM);
- (c) calculation of complex phase shifts, electric dipole matrix elements and solution of the multiple scattering problem (routine MSCALC);
- (d) calculation of the angular cross-section as in Eq. (1) (routine PHD).

3.1. Cluster potential

The coulombic potential and charge density of the cluster are calculated by means of the program VGEN in which relativistic atomic charge densities are generated (routine RHOAT) and overlapped by a monopole expansion (routine MOLPOT) and finally tailored (routine INPOT) according the choice of the muffin-tin radii to produce two files (called *coul.pot* and *rho.dens*) containing respectively the Coulomb potential and the charge density of the cluster under consideration on a radial mesh. An extract from the two files is given in the test run output. For a detailed description see Ref. [12]. The absorbing atom potential can be described by a “Z + 1” approximation or simply as a neutral atom (charelx=‘ex’ or ‘gs’ in the file input *msphd.inp*). The interstitial potential and charge density (vinp and rhoinp) can be different from the the quantity calculated because of the abrupt termination of the surface and for this reason they can be considered an input of the program, on the basis of charge densities obtained by total energy calculation.

The main routine (MSCALC) will calculate, on the basis of these two files, the HL energy-dependent exchange and correlation potential in order to calculate atomic phase-shifts at each new kinetic energy according to the approach of Hedin and Lundqvist [8]. This procedure incorporates the finite lifetime of the photoelectron in the final state and gives rise to a calculated mean free path. The muffin-tin radii are calculated according to two options (see the input file *msphd.inp*):

- (1) ‘stdcrm’: $R_i = R_{ij} / (1 + R_{nj} / R_{ni})$ where R_i is the muffin-tin radius for atom at site i , R_{ij} the distance between sites i and j and R_{ni} the Norman radius (enclosing a charge equal to $zato(i)$) for atom i . This is the default option;
- (2) ‘stdfac’ Norman radii scaled by a factor of 0.8. Finally radial matrix elements are calculated on the basis of the initial core state (core = ‘1s’, ‘2s’ and so on).

3.2. Symmetrized basis functions

The following step takes advantage of the symmetry of the system to reduce the size of the matrices. To do this a set of symmetrized basis functions is necessary. These basis functions are calculated by MOLSYM as a linear combination of real spherical harmonics centred at the equivalent sites. A set of files with the most recurrent symmetry operations is available with the code source. For the two test runs the *C4v.dat* and *Csx.dat* *C2v.dat* files are reported in test run input at the end of the paper. In the first line are given KTAU, INVER, and NREP (format (3I5)), i.e. the number of symmetry operations for the molecular group, the number of symmetry operations not involving inversion and the number of irreducible representations described in the file. In the following lines are given ID, OM, EGA, X, Y and Z (format (A10,F3.0,3X,F4.3,3F10.7)) a ten character identifier of the group operation, the angle of rotation $\text{OMEGA} = \text{OM} / \text{EGA}$ about the symmetry axis in units of π and the coordinates of any point on the rotation axis (or equivalently for reflections, the axis which defines the mirror plane). There are as many lines as symmetry operations. Then follows the description of the irreducible representation: NDIM (format (I5)), i.e. the representation dimension; TITLE (format (20A4)) an identifier for the irreducible representation. Then for each column of the first line of the matrix realization of the irreducible

representation: an identifier for the irreducible representation and the column of the transformation matrix (e.g., A1) (format (20A4)); the matrix element GAMMA(KT)(1,NCOL) (format (8F10.0)) of the matrix realization of the KTth symmetry operation of the irreducible representation of the symmetry group. They are listed 8 per line (DSRY(1,NCOL), . . . ,DSRY(8,NCOL), etc.). The basis functions are calculated up to the value of l_{\max} which can provide all the non zero t -matrices according to the criterion of the impact parameter, i.e. $l_{\max} = kR$ where R is the atomic radius. The symmetry files (extension *.sym*) are written for all the relevant irreducible representations of the point group [13] which are non-zero because of the dipole selection rule. An extract from the file is reported in the test run output (for a complete description refer to Ref. [12]).

3.3. Multiple scattering calculation

The third step is the calculation of atomic T-matrices (routine TMAT), and the solution of the multiple scattering problem (routine SMTX). The inversion of the linear system of equations is done using the NAG package [14] as external routines for inversion of symmetric double precision complex matrices to obtain the quantity of Eq. (3). The routines employed are F07QRF (Bunch–Kaufman factorization of complex symmetric matrix with packed storage adapted from LAPACK's ZSPTRF [15]) and F07QSF (solution of complex symmetric system of linear equations with multiple right-hand sides and matrix already factorized by F07QRF and packed storage adapted from LAPACK's ZSPTRS). The typical dimension of such a matrix is, in the most unfavorable case (no symmetries), $(l_{\max} + 1)^2 \times N_{\text{at}}$ of the order of 2500×2500 for a value of $l_{\max} = 4$ and 100 atoms in the cluster, which is the characteristic dimension for clusters at the surface sensitive kinetic energy (30–60 eV). The memory storage can be then estimated to be $1/2 \times 2500 \times 2500 = 50$ Mbyte because of the packed storage of the symmetric matrix. This memory allocation is nowadays easily affordable even with a personal computer. A brief description of the calculation is written in *mscal.log* file, where are reported the interstitial values of the potential and charge density, the value of the T-matrices for all the prototypical atoms of the cluster, and the value of the calculated mean free path. As a rule of thumb the cluster should have a radius of about twice the electron mean free path. All the multiple scattering calculation ingredients are stored in *.mat* files for every irreducible representation of interest to be used in the next steps of the calculation.

3.4. Angular cross section

The angular cross section is calculated by the routine PHD for the particular experimental geometry of the light source and the detection apparatus (subroutine POLARZ). This part of the task is computationally much lighter and can be accomplished independently once the scattering problem is solved (*icalcmode=1*). Experimental modes accessible in the code are the most usual ones (considered that the photon beam is fixed):

- (a) moving the sample (*imov=0*) by azimuthal and polar angle;
- (b) moving the detector (*imov=1*);
- (c) moving the detector along the polar scan while doing azimuthal scan rotating the sample around the surface normal (*imov=2*).

4. Input and output

A single input file *msphd.inp* is needed by the code, while symmetry files are provided with the code. Include files (extension *.inc*) for optimal dimensioning of the code is done automatically at each compilation. In the output file, the results will be printed in a 4 column file (*phd.plot*) for kinetic energy, polar angle, azimuthal angle, and intensity. In the case of several absorbing atoms the result will be appended one after the other. The general information about the execution of the calculation will be reported in *mscal.log*.

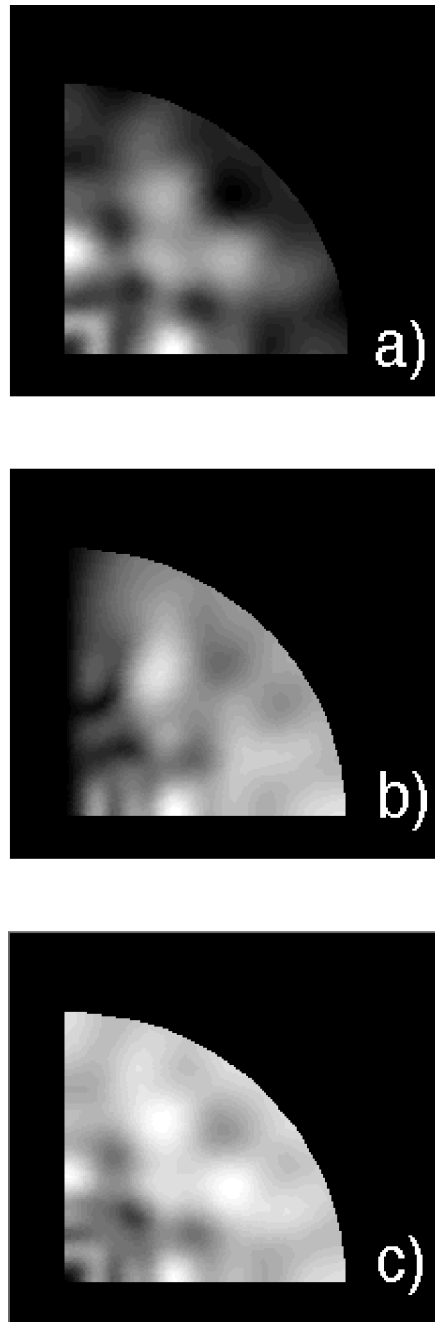


Fig. 1. The two-dimensional plots of simulated O/Ni(001) of the test case are reported: (a) motion of the sample; (b) motion of the detector; (c) motion of the detector along the polar angle and rotation of the sample around the normal to the surface. The polar angles from 0 to 80 and azimuthal from 0 to 90 (0 is the azimuthal angle corresponding to the x -axis of the surface unit cell of *msphd.inp* ([110])) are reported in a stereographic way.

5. Test run

We provide at the end of the paper two test runs for O 1s PD from $p2 \times 2$ -O/Ni(001) with fourfold symmetry, and that of Si 2p PD from the 2×1 -As/Si(001) surface, respectively. In the last case the fourfold symmetry is obtained by the double domain (2×1 and 1×2) of the reconstruction and by the two independent Si emitters. This is equivalent to having three more symmetry related emissions ($n_{\text{calc}}=3$) patterns which contribute to the final intensity. Furthermore in this second example the double emission from the second and half of the third plane of Si atoms is considered.

References

- [1] E.L. Bullock, R. Gunnella, L. Patthey, T. Abukawa, S. Kono, C.R. Natoli, L.S.O. Johansson, *Phys. Rev. Lett.* 74 (1995) 2571.
- [2] R. Gunnella, E.L. Bullock, L. Patthey, C.R. Natoli, T. Abukawa, S. Kono, L.S.O. Johansson, *Phys. Rev. B* 57 (1998) 14 739;
R. Gunnella, E.L. Bullock, C.R. Natoli, R.I.G. Uhrberg, L.S.O. Johansson, *Surf. Sci.* 352–354 (1996) 332.
- [3] C. Rojas, C. Polop, E. Román, J.A. Martín Gago, R. Gunnella, B. Brena, D. Cocco, G. Paolucci, *Phys. Rev. B* 57 (1998) 4493;
M. Rocca, L. Savio, L. Vattuone, U. Burghaus, V. Palomba, N. Novelli, F. Buatier de Mongeot, U. Valbusa, R. Gunnella, G. Comelli, A. Baraldi, S. Lizzit, G. Paolucci, *Phys. Rev. B* 61 (2000) 213.
- [4] K.-U. Weiss, R. Dippel, K.-M. Shindler, P. Gardner, V. Fritzsche, A.M. Bradshaw, A.L.D. Kilcoyne, D.P. Woodruff, *Phys. Rev. Lett.* 69 (1992) 3196.
- [5] L.J. Terminello, J.J. Barton, D.A. Lapiano-Smith, *Phys. Rev. Lett.* 70 (1993) 599.
- [6] X. Chen, D.K. Saldin, *Comput. Phys. Commun.* 112 (1998) 67;
G.R. Harp, Y. Ueda, X. Chen, D.K. Saldin, *Comput. Phys. Commun.* 112 (1998) 80;
X. Chen, G.R. Harp, Y. Ueda, D.K. Saldin, *Comput. Phys. Commun.* 112 (1998) 91.
- [7] C.R. Natoli, M. Benfatto, C. Brouder, M.F. Ruiz Lopez, D.L. Foulis, *Phys. Rev. B* 42 (1990) 1944.
- [8] L. Hedin, *Solid State Phys.* 23 (1969) 1; *J. Phys. C* 3 (1972) 73.
- [9] M. Biagini, *Phys. Rev. B* 48 (1993) 2974.
- [10] V. Fritzsche, *J. Phys: Condens. Matter* 2 (1990) 1413.
- [11] J.J. Rehr, R.C. Albers, *Phys. Rev. B* 41 (1990) 8139.
- [12] C.R. Natoli, *Operating Manual for Continuum*, unpublished. The code and the manual are available upon request by e-mail to natoli@Inf.infn.it.
- [13] M. Tinkham, *Group Theory and Quantum Mechanics*, McGraw-Hill, New York, 1964.
- [14] *NAG Fortran Library Manual – Mark 17*, The Numerical Algorithms Group Limited, 1995.
- [15] *LAPACK Package (version 3.0)*, Univ. of Tennessee, Univ. of California Berkeley, NAG Ltd., Courant Institute, Argonne National Lab., and Rice University.

Table 1

Input parameters

core	core level of photoemission (Ex. 1s, 2p _{3/2} , ...);
norman	criterium for choice of muffin-tin radius: (1) 'stdcrm': standard Norman criterion; (2) 'stdfac': Norman radii scaled by a factor of 0.8;
charelx	(1) 'ex': excited configuration for the absorbing atom; 'gs' atomic ground state;
emin	minimal electron kinetic energy (Ryd);
emax	maximal electron kinetic energy (Ryd);
estep	energy step for photon energy scan (Ryd);
lmax	max. value of angular momentum in the wave expansion;
vinp	interstitial coulombic potential (Ryd) (calculated if 0.0);
rhoinp	interstitial charge density (atomic u.) (calculated if 0.0);
cip	ionisation potential (Ryd);
fermi	fermi edge (Ry) (if 0.0 is calculated by the program);
teti, tetf, ntet	initial, final and step value of the internal polar angle (deg);
phii, phif, nphi	initial, final and step value of azimuthal angle (deg);
imov	0: moving sample; 1: moving detector; 2: moving detector along polar angle and sample about the normal to the surface (impinging light direction is fixed);
tetp, phip	the polar and azimuthal angle of X-ray beam when the detection is normal to the surface (deg);
epol	angle between the light electric field and normal to the incidence plane (deg);
icalcmode	calculation mode (0: total; 1: angular patterns only);
ai, aj, bi, bj	components of the two surface unit cell vectors (Å);
radius	maximum radius of scattering around each emitter (Å);
x(atom), y(atom)	x and y position of atom in the surface cell (units of surface cell vectors);
z(atom)	z position of atom (Å);
zato(atom)	atomic number of atom;
w(atom)	weight of the emitter (for multiemitter calculation);
sym(atom)	group of symmetry (<i>N</i> (no symmetry), C _{sy} , C _{sx} , C _{2v} , C ₂ , C _{3v} , C ₃ , C ₄ , C _{4v} , ...);
ncalc(atom)	for <i>n</i> symmetry related emitters on the surface is equal to <i>n</i> - 1. <i>n</i> - 1 lines must follow to provide couple of azimuthal angles related to phii, phif (see Appendix 2).

Appendix 1

TEST RUN INPUT #1

```

-----msphd.inp (starts next line) -----
c*****MSPHD.INP*****
&job
core='ls',
norman='stdcrm',
charelx='ex',
&end

***** Ni(001)p2x2-O*****
Computation of potential parameters
3.67 emin (minimal kin. energy(Ry))
3.67 emax (maximal kin. energy(Ry))
1. estep (energy step(Ry))
4 lmax (maximum value of l)
-0.0 vinp (inner coulombic potential(Ry) (calculated if 0.0))
0.0 rhoinp (interstitial charge density (atomic u.) (calculated if 0.0))
38.82 cip (ionisation potential(Ry))
-0.0 fermi (fermi edge(Ry) (calculated if 0.0))
0 teti (initial polar angle(deg))
85 tetf (final polar angle (deg))
41 ntet (number of polar angle calculation)
0. phii (initial azimuthal angle (deg))
360. phif (final azimuthal angle (deg))
121 nphi (number of azimuthal calculations)
0 imov (0/moving sample 1/moving detector 2/both)
135. tetp (polar angle of x-ray at detection normal (deg))
0. phip (azimuthal angle for x-ray incidence plane (deg))
90. epol (angle between e-field and normal to the incidence plane (deg))
0 icalcmode (calculation mode (0 full- 1 angular pattern))
*****cluster surface cell*****
*****x direction means azimuthal angle equal zero*****
4.978 0. ai,aj (components of unit cell vector (angstrom))
0.000 4.978 bi,bj (components of unit cell vector (angstrom))
7. radius (maximum radius of scattering (angstrom))
the x's and y's of the list are given in cell units the z's in angstrom;
w is the emitter contribution; ncalc is the number of symmetry related
emitters; ncalc lines follow the emitter line with related values of phii
and phif.
#atom x y z zato w sym ncalc (I3,3F9.5,2F7.3,A3,I3)
1 .25000 .25000 0.82000 8.0 1.000C4v 0
2 .00000 .00000 0.00000 28.0 0.000 N 0
3 .50000 .00000 0.00000 28.0 0.000 N 0
4 .00000 .50000 0.00000 28.0 0.000 N 0
5 .50000 .50000 0.00000 28.0 0.000 N 0
6 .25000 .25000 -1.76000 28.0 0.000 N 0
7 .25000 .75000 -1.76000 28.0 0.000 N 0
8 .75000 .25000 -1.76000 28.0 0.000 N 0
9 .75000 .75000 -1.76000 28.0 0.000 N 0

```

10	.00000	.00000	-3.52000	28.0	0.000	N	0
11	.50000	.00000	-3.52000	28.0	0.000	N	0
12	.00000	.50000	-3.52000	28.0	0.000	N	0
13	.50000	.50000	-3.52000	28.0	0.000	N	0
14	.25000	.25000	-5.28000	28.0	0.000	N	0
15	.25000	.75000	-5.28000	28.0	0.000	N	0
16	.75000	.25000	-5.28000	28.0	0.000	N	0
17	.75000	.75000	-5.28000	28.0	0.000	N	0

-----file ends previous line-----

-----C4v.dat (starts next line) -----

8	4	6					
	IDEN	2.	1.0	0.0	0.0	1.0	
	C2Z	1.	1.0	0.0	0.0	1.0	
	c4z	1.	2.0	0.0	0.0	1.0	
	c4-z	1.	-2.0	0.0	0.0	1.0	
	SGVx	1.	1.0	0.0	1.0	0.0	
	SGVy	1.	1.0	1.0	0.0	0.0	
	sgd1	1.	1.0	1.0	1.0	0.0	
	sgd2	1.	1.0	-1.0	1.0	0.0	
1	A1						
1.0		1.0	1.0	1.0	1.0	1.0	1.0
1	B1						
-1.0		1.0	1.0	-1.0	-1.0	1.0	1.0
-1.0		1.0	1.0	1.0	1.0	-1.0	-1.0
1	B2						
1.0		1.0	1.0	-1.0	-1.0	-1.0	1.0
1	E1						
0.0		1.0	-1.0	0.0	0.0	1.0	-1.0
1	E2						
1.0		0.0	0.0	1.0	-1.0	0.0	0.0
							-1.0

-----file ends previous line-----

TEST RUN OUTPUT #1

```

-----coul.pot-----
---
O      0 8 0 106 103   0.000000   0.000000   0.000000   1.589372   0.744000
2
 20   40   60   80  100  200  200  200  200  200
3
2.2133535E-03 4.4267070E-03 6.6400606E-03 8.8534141E-03 1.1066768E-02
4
-7.1954241E+03-3.5810097E+03-2.3762184E+03-1.7738373E+03-1.4124238E+03
5
-1.1714961E+03-9.9942031E+02-8.7037823E+02-7.7002667E+02-6.8975957E+02
6
...
Ni     028 0 130 127  -7.055293  -7.055293  -1.549576   2.470590   0.709000
27
 20   40   60   80  100  120  200  200  200  200
28
1.4577893E-03 2.9155787E-03 4.3733680E-03 5.8311574E-03 7.2889467E-03
29
-3.8153906E+04-1.8947160E+04-1.2545414E+04-9.3450557E+03-7.4253411E+03
30
-6.1460076E+03-5.2326462E+03-4.5480445E+03-4.0159672E+03-3.5906683E+03
31
-3.2430331E+03-2.9536490E+03-2.7090741E+03-2.4997056E+03-2.3184998E+03
32
-2.1601730E+03-2.0206839E+03-1.8968886E+03-1.7863048E+03-1.6869459E+03
33
-1.5157630E+03-1.3736160E+03-1.2537725E+03-1.1514239E+03-1.0630448E+03
34
-9.8599253E+02-9.1824761E+02-8.5824099E+02-8.0473540E+02-7.5674248E+02
35
-7.1346345E+02-6.7424596E+02-6.3855223E+02-6.0593504E+02-5.7601960E+02
36
...
Ni     1528 0   0 125   2.351764  -2.351764  -8.201412   2.289740   0.709000
509
Ni     1528 0   0 125  -2.351764   2.351764  -8.201412   2.289740   0.709000
510
Ni     1528 0   0 125   2.351764   2.351764  -8.201412   2.289740   0.709000
511
-1.4634909E-01
-----rho.dens-----
1.0526764E-02 4.0545911E-02 8.7931854E-02 1.5073537E-01 2.2715310E-01
27
3.1552223E-01 4.1429668E-01 5.2205429E-01 6.3747561E-01 7.5934830E-01
28
8.8655865E-01 1.0180768E+00 1.1529412E+00 1.2903260E+00 1.4293908E+00
29
1.5694593E+00 1.7098500E+00 1.8499607E+00 1.9892565E+00 2.1272517E+00
30

```

```

2.3976320E+00 2.6581112E+00 2.9063351E+00 3.1405646E+00 3.3594255E+00
31
3.5620372E+00 3.7478432E+00 3.9165597E+00 4.0681713E+00 4.2028625E+00
32
4.3209856E+00 4.4230334E+00 4.5096153E+00 4.5814403E+00 4.6392837E+00
33
4.6837860E+00 4.7159058E+00 4.7365655E+00 4.7466725E+00 4.7467395E+00
34
4.7212671E+00 4.6664531E+00 4.5887001E+00 4.4938213E+00 4.3869539E+00
35
...
8.1711593E-03

```

```

-----A1.sym-----
253 1
0 1 1
0 1 1 1.000000000
1 1 1
0 1 1 1.000000000
2 1 1
0 1 1 1.000000000
3 1 1
0 1 1 1.000000000
4 1 1
0 1 1 1.000000000
4 1 1
4 1 1 1.000000000
0 4 1
0 1 2 0.500000000 0 1 17 0.500000000 0 1 18 0.500000000 0 1 19
0.500000000
1 4 1
0 1 2 0.500000000 0 1 17 0.500000000 0 1 18 0.500000000 0 1 19
0.500000000
1 8 1
1 1 2 0.353553391 1-1 2 0.353553391 1 1 17 0.353553391 1-1
17-0.353553391
...

```

```

-----MSCALC.LOG-----
MSPHD.FOR
0 ***** Ni(001)p2x2-O*****

```

```

INITIAL EDGE =k
NUMBER OF CENTERS= 71
SYMMETRY INITIAL STATE LIN = 0
INTERSTITIAL COULOMB POT.=-0.1463491
INTERSTITIAL CHARGE DENS.= 0.0081712
natom= 1 l= 0 t1= 0.4880463E+00 -0.7976331E+00
natom= 1 l= 1 t1=-0.5528355E+00 -0.5073462E+00
natom= 1 l= 2 t1= 0.5158908E+00 -0.4776842E+00
natom= 1 l= 3 t1= 0.8933595E-01 -0.2119526E-01
natom= 1 l= 4 t1= 0.8456006E-02 -0.2096533E-02
natom= 2 l= 0 t1=-0.5681781E+00 -0.6850362E+00
natom= 2 l= 1 t1= 0.1829134E-01 0.8018755E-01

```

```

natom= 2 l= 2 t1= 0.3500119E+00 -0.1078675E+00
natom= 2 l= 3 t1= 0.4379539E+00 -0.5519684E+00
natom= 2 l= 4 t1= 0.1789217E+00 -0.9448394E-01
natom= 3 l= 0 t1=-0.5729338E+00 -0.6757189E+00
natom= 3 l= 1 t1= 0.3336918E-01 0.8191770E-01
natom= 3 l= 2 t1= 0.3725227E+00 -0.1251382E+00
natom= 3 l= 3 t1= 0.4358172E+00 -0.5846277E+00
natom= 3 l= 4 t1= 0.1850654E+00 -0.9883929E-01
natom= 4 l= 0 t1=-0.5829354E+00 -0.6726038E+00
natom= 4 l= 1 t1= 0.6966541E-01 0.8664814E-01
natom= 4 l= 2 t1= 0.4133911E+00 -0.1652071E+00
natom= 4 l= 3 t1= 0.4265232E+00 -0.6263158E+00
natom= 4 l= 4 t1= 0.1631327E+00 -0.8019042E-01

```

...

INTERSTITIAL VCON = (-0.447508, 0.261106) - FERMİ LEVEL = -0.186499

ENERGY	TOTAL MFP	INT. MFP	M.T. MFP
3.67000	5.09939	4.11314	9.79261

...

INITIAL POLARIZATION Ex = 0.70711 Ey = 0.00000 Ez = 0.70711

-----phd.plot-----

.....

3.6700001	0.0000000	357.0000000	0.0260717	0.0000000
3.6700001	0.0000000	360.0000000	0.0260717	0.0000000
3.6700001	2.1250000	0.0000000	0.0287559	0.0000000
3.6700001	2.1250000	3.0000000	0.0287520	0.0000000
3.6700001	2.1250000	6.0000000	0.0287397	0.0000000
3.6700001	2.1250000	9.0000000	0.0287198	0.0000000
3.6700001	2.1250000	12.0000000	0.0286932	0.0000000
3.6700001	2.1250000	15.0000000	0.0286612	0.0000000
3.6700001	2.1250000	18.0000000	0.0286250	0.0000000

.....

Appendix 2

TEST RUN INPUT #2

```

-----msphd.inp (starts next line) -----
c*****MSPHD.INP*****
&job
core='2p1/2',
norman='stdcrm',
charelx='ex',
&end
*****2x1-As/Si(001) *****
Computation of potential parameters
1.80 emin (minimal kin. energy(Ry))
1.80 emax (maximal kin. energy(Ry))
1. estep (energy step(Ry))
2 lmax (maximum value of l)
-0.0 vinp (inner coulombic potential(Ry) (calculated if 0.0))
0.0 rhoinp (interstitial charge density (atomic u.) (calculated if 0.0))
7.28 cip (ionisation potential(Ry))
-0.0 fermi (fermi edge(Ry) (calculated if 0.0))
45 teti (initial polar angle(deg))
45 tetf (final polar angle (deg))
1 ntet (number of polar angle calculation)
-60. phii (initial azimuthal angle (deg))
60. phif (final azimuthal angle (deg))
61 nphi (number of azimuthal calculations)
0 imov (0/moving sample 1/moving detector 2/both)
135. tetp (polar angle of x-ray at detection normal (deg))
0. phip (azimuthal angle for x-ray incidence plane (deg))
90. epol (angle between e-field and normal to the incidence plane (deg))
0 icalcmode (calculation mode (0 full- 1 angular pattern))
*****cluster surface cell*****
*****x direction corresponds to azimuthal angle equal zero*****
7.68 0. ai,aj (components of unit cell vector (angstrom))
0.000 3.84 bi,bj (components of unit cell vector (angstrom))
4. radius (maximum radius of scattering (angstrom))
the x's and y's of the list are given in cell units the z's in angstrom;
w is the emitter contribution; ncalc is the number of symmetry related
emitters; ncalc lines follow the emitter line with related values of phii
and phif.
#atom x y z zato w sym ncalc (I3,3F9.5,2F7.3,A3,I3)
1 .01400 .00000 -1.43000 14.0 1.000Cs 3
120. 240.
30. 150.
210. 330.
2 .48600 .00000 -1.43000 14.0 0.000 N 0
3 .08500 .50000 -0.00000 33.0 0.000 N 0
4 .41500 .50000 -0.00000 33.0 0.000 N 0
5 .25000 .00000 -2.91100 14.0 0.000 N 0
6 .75000 .00000 -2.70400 14.0 1.000C2v 3
120. 240.

```

30. 150.

210. 330.

7	.25000	.50000	-4.21100	14.0	0.000	N	0
8	.75000	.50000	-4.03100	14.0	0.000	N	0
9	.00000	.00000	-5.43000	14.0	0.000	N	0
10	.50000	.00000	-5.43000	14.0	0.000	N	0
11	.00000	.50000	-6.78700	14.0	0.000	N	0
12	.50000	.50000	-6.78700	14.0	0.000	N	0

-----file ends previous line-----

-----Csx.dat (starts next line) -----

2	1	2					
	IDEN	2.	1.0	0.0	0.0	1.0	
	SIGx	1.	1.0	0.0	1.0	0.0	
1	A1						
		1.0	1.0				
1	A2						
		1.0	-1.0				

-----file ends previous line-----

-----C2v.dat (starts next line) -----

4	2	4					
	IDEN	2.	1.0	0.0	0.0	1.0	
	C2Z	1.0	1.0	0.0	0.0	1.0	
	SGVx	1.	1.0	0.0	1.0	0.0	
	SGVy	1.	1.0	1.0	0.0	0.0	
1	A1						
		1.0	1.0	1.0	1.0		
1	A2						
		1.0	1.0	-1.0	-1.0		
1	B1						
		1.0	-1.0	1.0	-1.0		
1	B2						
		1.0	-1.0	-1.0	1.0		

-----file ends previous line-----

TEST RUN OUTPUT #2

```
-----phd.plot-----  
...  
 1.8000000  45.0000000  -30.0000000  1.5953791  0.0000000  
 1.8000000  45.0000000  -28.0000000  1.5529697  0.0000000  
 1.8000000  45.0000000  -26.0000000  1.5287992  0.0000000  
 1.8000000  45.0000000  -24.0000000  1.5195979  0.0000000  
 1.8000000  45.0000000  -22.0000000  1.5215156  0.0000000  
 1.8000000  45.0000000  -20.0000000  1.5307260  0.0000000  
 1.8000000  45.0000000  -18.0000000  1.5436525  0.0000000  
 1.8000000  45.0000000  -16.0000038  1.5570811  0.0000000  
 1.8000000  45.0000000  -14.0000038  1.5682749  0.0000000  
 1.8000000  45.0000000  -12.0000000  1.5751499  0.0000000  
 1.8000000  45.0000000  -10.0000000  1.5764984  0.0000000  
...  
 1.8000000  45.0000000  -30.0000000  0.2878717  0.0000000  
 1.8000000  45.0000000  -28.0000000  0.2887921  0.0000000  
 1.8000000  45.0000000  -26.0000000  0.2981655  0.0000000  
 1.8000000  45.0000000  -24.0000000  0.3153667  0.0000000  
 1.8000000  45.0000000  -22.0000000  0.3384925  0.0000000  
 1.8000000  45.0000000  -20.0000000  0.3645651  0.0000000  
 1.8000000  45.0000000  -18.0000000  0.3900904  0.0000000  
 1.8000000  45.0000000  -16.0000038  0.4117952  0.0000000  
 1.8000000  45.0000000  -14.0000038  0.4272811  0.0000000  
 1.8000000  45.0000000  -12.0000000  0.4353821  0.0000000  
 1.8000000  45.0000000  -10.0000000  0.4362352  0.0000000  
...  
-----
```