A MODIFIED GREEN'S FUNCTION TECHNIQUE FOR THE
CALCULATION OF LATTICE DISTORTION
SURROUNDING INTERSTITIALS

by

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ABSTRACT

The Green's function technique for the calculation of lattice distortion surrounding point defects is modified to enable the treatment of interstitial defects. The modification consists in treating a selected region immediately surrounding the interstitial formally as a cluster of $n+1$ interstitials and n vacancies. This region, called the interstitial "core", includes atoms which are displaced by large amounts from their normal lattice sites and therefore cannot be treated within the standard harmonic approximation. The method is illustrated by a calculation for the $[111]$ split crowdion configuration in tungsten. Displacement fields are calculated for two separate interatomic potentials, one fitted to the phonon spectrum and the other to elastic constants. Predicted atomic relaxations for both potentials are quite similar.

I. INTRODUCTION

The techniques used in atomistic calculations of lattice strain surrounding point defects may roughly be divided into two categories. The first of these consists of methods which are formulated entirely in real space. A variety of such techniques, both of the "static" and of the dynamic "computer simulation" types, have been developed in recent years⁽¹⁾.

The real space methods have in common the practical limitation of becoming somewhat cumbersome when applied to a crystallite consisting of more than a few hundred atoms. This is particularly a problem for certain types of point defects with large defect "strength".

The other category comprises those methods which rely to some extent on reciprocal space techniques. The latter are often referred to as "lattice statics", borrowing somewhat in their formulation from the theory of lattice dynamics. Introduced by Matsubara⁽²⁾ in connection with the problem of diffuse x-ray scattering by point defects, lattice statics was further developed by Kanzaki⁽³⁾ and by Hardy and co-workers⁽⁴⁾. Recently the method has been recast in terms of lattice Green's functions by Tewary and Bullough^(5,5a). A useful feature of the Green's function approach is that it allows the point group symmetry of the defect to be exploited in a natural and systematic way.

The method of lattice statics is characterized by a second order expansion of the crystal energy in the atomic displacements (the harmonic approximation) and the application of periodic boundary conditions. This procedure enables a decoupling of the equations of

equilibrium in such a way that the size of the matrices to be inverted is determined by the range of interatomic interaction rather than the size of the crystal being considered. One is therefore able to treat an effectively infinite crystal.

A difficulty with lattice statics is that for certain defects, such as interstitials, the relaxation of near neighbors is large so that the harmonic approximation is not reliable. In the present work we suggest how this difficulty may be dealt with within the Green's function formulation of lattice statics. The basic idea is first to displace certain near neighbor atoms to positions close to their final equilibrium and only then to apply the harmonic approximation. In this approach a self-interstitial is treated formally as a cluster of $n+1$ "interstitials" and n "vacancies" where n may typically be of order 10 or 20. The "initial" positions of the near neighbor atoms corresponding approximately to a minimum energy configuration have to be determined in a separate calculation.

To illustrate this method, it is applied to a case in which the lattice distortion is particularly severe, namely that of the split crowdion configuration in bcc tungsten. Displacement fields are calculated for two different interatomic potentials.

The displacement field of an interstitial has an important bearing on a number of physical properties, e.g. interstitial formation energy and volume, diffusion, internal friction and diffuse x-ray scattering. Recently its effect on field ion microscope image contrast has been investigated⁽⁶⁾. Some of these properties will be discussed in a sequel to the present paper.

In this paper, however, consideration is confined to the calculation of lattice distortion.

In section II we review the Green's function formulation of lattice statics and outline briefly how one may evaluate the various parameters arising in the theory. In section III we consider the modifications necessary for the treatment of the crowdion configuration. Finally, in section IV results are presented and discussed.

II. GREEN'S FUNCTION FORMALISM

The Green's function approach to the calculation of lattice distortion surrounding defects is discussed in considerable detail in reference (5) and therefore the following discussion, which is intended to provide a framework for the modifications introduced in section III, is somewhat abbreviated. Consider the case of an isolated point defect imbedded in a Bravais lattice consisting of N atoms. In the following one may think either of the surface atoms as being fixed or of the N atom cell repeating itself in a periodic superlattice.

In the harmonic approximation one writes the crystal energy as

$$\Phi = \Phi_0 - \sum_{\ell\alpha} F_{\alpha}(\ell) u_{\ell\alpha} + \frac{1}{2} \sum_{\substack{\ell\alpha \\ \ell'\beta}} \phi_{\alpha\beta}(\ell, \ell') u_{\ell\alpha} u_{\ell'\beta} \quad (2.1)$$

where $\vec{u}_{\ell} = \vec{r}_{\ell} - \vec{R}_{\ell}$ is the displacement vector of the ℓ^{th} atom from its normal lattice position. The equations of static equilibrium are

$$\begin{aligned} \frac{\partial \Phi}{\partial u_{\ell\alpha}} &= -F_{\alpha}(\ell) + \sum_{\beta\ell'} \phi_{\alpha\beta}(\ell, \ell') u_{\ell'\beta} = 0 \\ \ell &= 1, 2, \dots, N, \\ \alpha &= 1, 2, 3 \end{aligned} \quad (2.2)$$

In matrix notation this may be written

$$\phi u = F$$

where ϕ is a $3N$ dimensional square matrix and u and F are $3N$ dimensional column vectors. A formal solution to this equation is given by

$$u = (\phi)^{-1} F = G F \quad (2.3)$$

where G is the static Green's function.

It is convenient to decompose ϕ into two contributions:

$$\phi = \phi^0 - \delta\phi \quad (2.4)$$

In the case of an interstitial, ϕ^0 corresponds to a perfect lattice in which a hypothetical "noninteracting" interstitial has been placed. $-\delta\phi$ is the change in ϕ which occurs upon "turning on" the interstitial-lattice interactions[†]. With the use of equation (2.4) the Green's function can be written

$$\begin{aligned} G &= (1 - G^0 \delta\phi)^{-1} G^0 \\ &= G^0 + G^0 \delta\phi G \end{aligned} \quad (2.5)$$

where $G^0 \equiv (\phi^0)^{-1}$ is the Green's function for the perfect lattice.

If one assumes that the interatomic forces are of finite range, for example extending only to first or second nearest neighbors, then a considerable simplification of equation (2.5) can be achieved through matrix partitioning⁽⁷⁾. One can write $\delta\phi$ in the form

$$\delta\phi = \begin{pmatrix} \delta\phi^p & 0 \\ 0 & 0 \end{pmatrix}$$

where the dimension of $\delta\phi^p$ is $3n_p$, n_p-1 being equal to the number of atoms interacting directly with the interstitial. The atoms counted in n_p comprise what is called the "perturbed space"⁽⁵⁾. If G^0 and G are similarly partitioned, i.e.

$$G^0 = \begin{pmatrix} g^0 & G_{12}^0 \\ G_{21}^0 & G_{22}^0 \end{pmatrix}$$

[†]In the case of a split interstitial a "vacancy" is created at the center of mass of the split pair and so in this case one must also "turn off" the vacant site-lattice atoms interactions.

$$G = \begin{pmatrix} g & G_{12} \\ G_{21} & G_{22} \end{pmatrix}$$

equation (2.5) reduces to the four matrix equations

$$g = g^0 + g^0 \delta\phi^P g \quad (2.6)$$

$$G_{12} = G_{12}^0 + g^0 \delta\phi^P G_{12} \quad (2.7)$$

$$G_{21} = G_{21}^0 + G_{21}^0 \delta\phi^P g \quad (2.8)$$

$$G_{22} = G_{22}^0 + G_{21}^0 \delta\phi^P G_{12} \quad (2.9)$$

Equation (2.6), which governs the displacements for the perturbed space, is the key to this set of equations; once it has been solved G_{12} , G_{21} and G_{22} can easily be evaluated. G_{21} determines the displacement field outside the perturbed space. Thus if u and F are partitioned as $u \equiv \begin{pmatrix} u^P \\ U \end{pmatrix}$, $F \equiv \begin{pmatrix} f \\ 0 \end{pmatrix}$, one has

$$u^P = gf \quad (2.10)$$

$$U = G_{21} f \quad (2.11)$$

The Green's function equations have a close parallel in the formulation of lattice statics of Kanzaki⁽³⁾. Using equations (2.3) and (2.5), one can write

$$\begin{aligned} u &= G_0 (1 + \delta\phi G) F \\ &= G_0 (F + \delta\phi u) \equiv G_0 F^* \end{aligned}$$

where F^* may be identified with the "force" in the Kanzaki approach. In partitioned form these equations become

$$u^p = g^o f^* \quad (2.12)$$

$$U = G_{21}^o f^* \quad (2.13)$$

where $f^* = f + \delta\phi^p u^p$.

It may be mentioned that Flinn and Maradudin⁽⁸⁾ developed a Green's function approach similar to that outlined here. These authors have approximated equation (2.6) by $g = g^o + g^o \delta\phi^p g^o$. This is a justifiable procedure if the lattice distortion is sufficiently small. This limitation, however, effectively restricts its application to the cases of vacancies and substitutional impurities and even for these defects it may not be sufficiently accurate⁽⁹⁾.

In the presence of an isolated point defect a crystal in general retains part or all of its point group symmetry around the defect site. With the help of group theoretical methods, as discussed in reference (5), this symmetry enables one to deal with an equation analogous to (2.6) but of greatly reduced dimension,

$$u^r = g^r f^r \quad (2.14)$$

where

$$\begin{aligned} g^r &= g^{or} + g^{or} \delta\phi^{pr} g^r \\ &= (1 - g^{or} \delta\phi^{pr})^{-1} g^{or} \end{aligned} \quad (2.15)$$

A "reduced" matrix M^r (i.e. g^{or} , $\delta\phi^{pr}$ or g^r) is defined by

$$M_{ij}^r = \sum_{\alpha\beta} \psi_{\alpha}^i(\ell) M_{\alpha\beta}(\ell, \ell') \psi_{\beta}^j(\ell).$$

Here the quantities ψ^i are the basis vectors of the identity representation of the point group of the defect. These vectors

belong to the perturbed space and are of dimension $3n_p$. Reduced force and displacement vectors are defined

$$F_i^r = \sum_{\alpha} \psi_{\alpha}^i(\ell) F_{\alpha}(\ell),$$

$$u_i^r = \sum_{\alpha} \psi_{\alpha}^i(\ell) u_{\alpha}(\ell).$$

The real space displacements are related to the corresponding reduced space quantities by the inversion formula

$$u_{\alpha}(\ell) = \sum_{i=1}^{n_r} u_i^r \psi_{\alpha}^i(\ell) \quad (2.16)$$

where n_r , the dimension of the reduced space, is equal to the multiplicity of the identity representation in the decomposition of the "total representation" of the perturbed space⁽⁵⁾.

To perform an explicit calculation based on the Green's function method one requires the zero-order Green's function G^0 and the pairwise interaction potential $v(r)$ between atoms from which the force vector F may be obtained. The former may be expressed in the form

$$G^0(\ell, \ell') = \sum_{\vec{k}} [\phi^0(\vec{k})]^{-1} e^{i\vec{k} \cdot (\vec{R}_{\ell} - \vec{R}_{\ell'})} \quad (2.17)$$

where the sum is over $\vec{k}$ vectors in the first Brillouin zone and

$$\phi^0(\vec{k}) = \sum_{\ell} \phi(\ell) e^{-i\vec{k} \cdot \vec{R}_{\ell}}$$

is the dynamical matrix of the perfect lattice. The inverse of $\phi^0(\vec{k})$ can be calculated either from interatomic force constants fitted to the experimental phonon spectra⁽⁵⁾ or by a more direct

fitting procedure^(5a). The mesh spacing chosen for the summation in equation (2.17) corresponds to the size of the lattice crystallite being considered⁽¹⁰⁾. For an infinite lattice the sum is replaced by an integral. An efficient procedure based on Gaussian quadrature for the evaluation of such integrals has been developed by Boyer and Hardy⁽¹¹⁾.

The interatomic potential $v(r)$ may be obtained via pseudopotential calculations where applicable or through semiempirical fitting procedures^(11,12). These methods have somewhat more theoretical justification than older Morse or Rydberg potential techniques.

III. APPLICATION TO [111] SPLIT CROWDION

In applying the Green's function technique discussed above to interstitial defects one runs into difficulties because of the large displacements of near neighbors. To consider a specific example, the nearest neighbors to the [111] split crowdion configuration in bcc metals are displaced by about $.5a$ (a being half the lattice constant). A very rough upper bound on the range of validity of the harmonic approximation, equation (2.1), is furnished by the Lindemann melting criterion⁽¹³⁾. For a bcc crystal the rms vibration amplitude at melting is about $.25a$. The expansion in equation (2.1) must be considered suspect for atoms displaced by amounts comparable to or greater than this value.

To remove this difficulty equation (2.1) may be modified in the following way. Assume that one has an independent estimate of approximate equilibrium positions $\vec{R}_\ell$ of the n_c atoms (including the interstitial) whose displacements are "large". One defines $\vec{u}_\ell = \vec{r}_\ell - \vec{R}_\ell$ for these atoms which are referred to as the interstitial "core". The expansion parameters $\vec{u}_\ell$ are then small and the calculation may be carried out as discussed below. The core atoms are treated as "noninteracting" in the calculation of ϕ_0 ; $\delta\phi$ is evaluated with the core-core and core-lattice interactions "turned on" and the interactions between lattice atoms and the "vacancies" left by the displacement of the core atoms "turned off". In this treatment the core can be thought of as consisting of n_c interstitials and $n_c - 1$ vacancies.

Displacement field calculations have been performed for the [111] split crowdion configuration in tungsten using two different

interatomic potentials. One of these was fitted to the phonon spectrum[†] and the other, developed by Johnson and Wilson⁽¹¹⁾, to the elastic constants. These potentials, labeled I and II respectively, are plotted in Figure 1.

The selected core region for the present calculations is illustrated in Figure 2. For the crowdion configuration the atoms along the interstitial axis undergo the largest displacements. The core region indicated in the figure consists of 10 interstitials and 9 vacancies. 62 lattice atoms interact directly with the core so that the entire perturbed space consists of 72 atoms. The appropriate point group for the crowdion configuration is isomorphic to the point group denoted L in electronic band theory⁽¹⁴⁾. The identity representation of this group contains 26 basis vectors in the perturbed space.

The perturbed space Green's function g^0 may be written in the form

$$g^0 = \begin{pmatrix} g^{oc} & 0 \\ 0 & g^{ol} \end{pmatrix}$$

Here g^{oc} is a 30x30 matrix whose elements are given by

$$g_{\alpha\beta}^{oc}(\ell, \ell') = r \delta_{\alpha\beta} \delta_{\ell\ell'}$$

where ℓ and ℓ' run over atoms within the core and $r = \lim_{\omega \rightarrow 0} \frac{1}{m\omega^2}$ is the free particle Green's function⁽⁵⁾.

[†]This potential will be discussed more fully in a future paper.

$$G_{\alpha\beta}^{01}(\ell, \ell') = G_{\alpha\beta}^0(\ell - \ell')$$

is a 186x186 dimensional matrix corresponding to the remaining part of the perturbed space. $\delta\phi^P$ may be written

$$\delta\phi^P = \begin{pmatrix} \delta\phi^C & \delta\phi^{C1} \\ \delta\phi^{C1} & \delta\phi^1 \end{pmatrix}$$

where

$$\begin{aligned} \delta\phi_{\alpha\beta}^C(\ell, \ell') &= (1 - \delta_{\ell\ell'}) \{ [\kappa_r(|\vec{R}_\ell - \vec{R}_{\ell'}|) - \kappa_t(|\vec{R}_\ell - \vec{R}_{\ell'}|)] C_\alpha(\ell - \ell') C_\beta(\ell - \ell') \\ &\quad + \kappa_t(|\vec{R}_\ell - \vec{R}_{\ell'}|) \delta_{\alpha\beta} \} + \delta_{\ell\ell'} \sum_c \{ [\kappa_t(|\vec{R}_\ell - \vec{R}_{\ell''}|) \\ &\quad - \kappa_r(|\vec{R}_\ell - \vec{R}_{\ell''}|)] C_\alpha(\ell - \ell'') C_\beta(\ell - \ell'') - \kappa_t(|\vec{R}_\ell - \vec{R}_{\ell''}|) \delta_{\alpha\beta} \} \\ &\quad + \delta_{\ell\ell'} \sum_l \{ [\kappa_t(|\vec{R}_\ell - \vec{R}_{\ell''}|) - \kappa_r(|\vec{R}_\ell - \vec{R}_{\ell''}|)] C_\alpha(\ell - \ell'') C_\beta(\ell - \ell'') \\ &\quad - \kappa_t(|\vec{R}_\ell - \vec{R}_{\ell''}|) \delta_{\alpha\beta} \} \end{aligned} \quad (3.1)$$

$$\begin{aligned} \delta\phi_{\alpha\beta}^{C1}(\ell, \ell') &= [\kappa_r(|\vec{R}_\ell - \vec{R}_{\ell'}|) - \kappa_t(|\vec{R}_\ell - \vec{R}_{\ell'}|)] C_\alpha(\ell - \ell') C_\beta(\ell - \ell') \\ &\quad + \kappa_t(|\vec{R}_\ell - \vec{R}_{\ell'}|) \delta_{\alpha\beta} \end{aligned} \quad (3.2)$$

$$\delta\phi_{\alpha\beta}^{C1}(\ell, \ell') = \delta\phi_{\beta\alpha}^{C1}(\ell', \ell) \quad (3.3)$$

$$\begin{aligned} \delta\phi_{\alpha\beta}^1(\ell, \ell') &= \delta_{\ell\ell'} \{ \sum_c [\kappa_t(|\vec{R}_{\ell''} - \vec{R}_\ell|) - \kappa_r(|\vec{R}_{\ell''} - \vec{R}_\ell|)] C_\alpha(\ell - \ell'') C_\beta(\ell - \ell'') \\ &\quad - \kappa_t(|\vec{R}_{\ell''} - \vec{R}_\ell|) \delta_{\alpha\beta} + \sum_v [\kappa_r(|\vec{R}_{\ell''} - \vec{R}_\ell|) \\ &\quad - \kappa_t(|\vec{R}_{\ell''} - \vec{R}_\ell|)] C_\alpha(\ell - \ell'') C_\beta(\ell - \ell'') \\ &\quad + \kappa_t(|\vec{R}_{\ell''} - \vec{R}_\ell|) \delta_{\alpha\beta} \} \end{aligned} \quad (3.4)$$

In equations (3.1-3.4) $\kappa_t(r) = \frac{dv(r)}{dr}/r$, the tangential force constant; $\kappa_r(r) = \frac{d^2v(r)}{dr^2}$, the radial force constant; $C_\alpha(\ell-\ell'')$ is the α^{th} directional cosine of the vector joining the ℓ^{th} and ℓ'^{th} atoms; $\sum'_c$ denotes a sum over core atoms, in which the prime indicates atom ℓ is omitted; $\sum_l$ is a sum over lattice atoms and $\sum_v$ over core vacancies.

Lattice Green's functions for tungsten were evaluated with the help of equation (2.17), using a two nearest neighbor force constant model. The force constants were those used in constructing potential I. A simple cubic mesh including 54,000 points in the first Brillouin zone was employed in this calculation. Numerical results for the first several neighbors are listed in Table 1. Very similar values were obtained for Green's functions determined from force constants based on potential II.[†]

The only input to the full calculation not yet discussed is the "initial" configuration of the interstitial core atoms. This may be obtained, for example, by performing a preliminary relaxation calculation for near neighbor shells. In this, one relaxes one shell at a time holding the rest of the lattice fixed; this process may be iterated until one is reasonably close to the final equilibrium positions. Alternatively the initial core configuration may be taken from a previously calculated displacement field obtained for a

[†]This is actually to be expected in spite of the apparent dissimilarity in the two potentials. The static lattice Green's functions are governed mainly by the continuum limit of the phonon spectrum i.e. by the elastic constants (5a). The predictions of both potentials are similar in this limit.

similar interatomic potential. It is worth remarking here that the choice of atoms to be included in the interstitial core can only be justified a posteriori. If the final calculated displacements of all atoms outside the core are sufficiently small (i.e. $\lesssim 0.05a$) then the selection of atoms to be included within the core may be considered satisfactory.

IV. RESULTS AND DISCUSSION

The relaxed positions of 40 shells of atoms in the vicinity of the interstitial are given in Table 2. Values are presented for both interatomic potentials shown in Figure 1. Displacements for the perturbed space (consisting of the first 16 shells) were determined with the use of equations (2.14-2.16), while those of atoms outside the perturbed space were evaluated with the help of equation (2.13).

In obtaining the results given in Table 2, several iterations of equation (2.15) were performed. By solving this equation for a given core configuration one obtains calculated values for core displacements which are then the basis for a new calculation with a revised core configuration. This process may be repeated until one is satisfied that the "initial" core configuration is sufficiently close to the equilibrium configuration or in other words until the core displacements u_c are sufficiently small. In the present calculation the criterion $u_c \leq 0.01a$ for core atoms was adopted. How many iterations are necessary to achieve this depends on the configuration for the initial iterative cycle but in general the process is rapidly convergent and usually two or three iterations are sufficient.

The selection of 10 interstitials and 9 vacancies as the core region may perhaps be considered conservative; calculated perturbed space displacements for a core consisting of 8 interstitials and 7 vacancies are mostly within 20% of those given in Table 2. The size of the core one selects depends on the accuracy that is desired.

By comparing the displacements for the 2 potentials in Table 2, one observes that on the whole values are quite close. Apparently the magnitude of these displacements is determined more by the fact that a strong hard core repulsion exists at distances just below the nearest neighbor separation than by the exact details of the potential "well" in the vicinity of the first two nearest neighbors.

An interesting question is at what distance from the defect does the displacement field approach the asymptotic inverse square behavior predicted by elasticity theory. This matter could be investigated by combining the present approach with the treatment adopted by Flocken and Hardy⁽¹⁵⁾ in their studies of the asymptotic displacement field of vacancies. This has not been undertaken as yet. However, judging from the results of the above mentioned authors one would surmise that the elastic limit is not approached for several tens of shells from the defect in any given direction.

Finally, a point which perhaps is obvious but may be overlooked concerning the question of metastable configurations. The Greens function technique does not guarantee that one will arrive at the configuration of minimum energy consistent with a given point group symmetry. Rather, it allows one to calculate in an approximate way the extremal configuration "closest" to the initial configuration. In any given case the possibility that the former is metastable cannot be entirely ruled out. In most case of interest, however, it is not unreasonable to assume that one arrives, by the method we have described, at the lowest energy configuration for a given symmetry.

In closing, it is worth taking note of the "modified lattice statics" technique developed recently by Flocken⁽¹⁶⁾. In several respects Flocken's method is similar to the Green's function approach discussed here. For example, equation (4) in reference (15) is analogous to our equations (2.12) and (2.13). One important difference, however, is that the Green's function approach allows one to relax the defect core and the surrounding lattice simultaneously which is not possible in the "modified lattice statics" method.

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TABLE 1

Static Green's functions for tungsten calculated using
2 nearest neighbor force constant model consistent with
potential I. (units: 10^{-5} cm/dyne)

ℓ	$G^{\circ}_{11}(\ell)$	$G^{\circ}_{22}(\ell)$	$G^{\circ}_{33}(\ell)$	$G^{\circ}_{23}(\ell)$	$G^{\circ}_{13}(\ell)$	$G^{\circ}_{12}(\ell)$
000	.49506	.49506	.49506	0	0	0
111	.12696	.12696	.12696	.02263	.02263	.02263
200	.15355	.08815	.08815	0	0	0
220	.07357	.07357	.06023	0	0	.01144
311	.07597	.05207	.05207	.00227	.00768	.00768
222	.05886	.05886	.05886	.01065	.01065	.01065
400	.07142	.03907	.03907	0	0	0
420	.05178	.03787	.03409	0	0	.00706
331	.04504	.04504	.03660	.00302	.00302	.00852
422	.04436	.03352	.03352	.00290	.00613	.00613
333	.03476	.03476	.03476	.00607	.00607	.00607
511	.04788	.02842	.02842	.00051	.00326	.00326
440	.03274	.03274	.02485	0	0	.00685
531	.03513	.02705	.02367	.00113	.00204	.00590
442	.02978	.02978	.02457	.00309	.00309	.00614
600	.04266	.02255	.02255	0	0	0
620	.03635	.02235	.02095	0	0	.00405
533	.02887	.02297	.02297	.00265	.00459	.00459
622	.03264	.02077	.02077	.00107	.00358	.00358
444	.02307	.02307	.02307	.00416	.00416	.00416
711	.03264	.01755	.01755	.00019	.00172	.00172
551	.02380	.02380	.01770	.00109	.00109	.00548
640	.02656	.02095	.01715	0	0	.00515
642	.02465	.01963	.01702	.00150	.00237	.00471
553	.02075	.02075	.01734	.00271	.00271	.00457

731	.02679	.01718	.01560	.00050	.00131	.00389
800	.02895	.01428	.01428	0	0	0
733	.02308	.01533	.01533	.00128	.00322	.00322
644	.02004	.01637	.01637	.00230	.00356	.00356
820	.02635	.01422	.01358	0	0	.00247
660	.01852	.01852	.01300	0	0	.00469
822	.02440	.01351	.01351	.00050	.00225	.00225
555	.01624	.01624	.01624	.00317	.00317	.00317
751	.01995	.01603	.01265	.00059	.00087	.00435
662	.01752	.01752	.01292	.00143	.00143	.00437
840	.02108	.01376	.01174	0	0	.00368
753	.01780	.01445	.01247	.00155	.00225	.00377
911	.02358	.01140	.01140	.00009	.00105	.00105
842	.01985	.01311	.01169	.00079	.00172	.00343
664	.01495	.01495	.01257	.00232	.00232	.00354
931	.02055	.01127	.01043	.00026	.00088	.00262

TABLE 2

Relaxed atomic positions surrounding [111] split crowdion
in tungsten calculated for two interatomic potentials.
The first 16 shells comprise the perturbed space (units: a)

ℓ	POTENTIAL I			POTENTIAL II		
	$r_1(\ell)$	$r_2(\ell)$	$r_3(\ell)$	$r_1(\ell)$	$r_2(\ell)$	$r_3(\ell)$
xxx	0.435	0.435	0.435	0.437	0.437	0.437
111	1.311	1.311	1.311	1.320	1.320	1.320
222	2.186	2.186	2.186	2.211	2.211	2.211
333	3.101	3.101	3.101	3.127	3.127	3.127
444	4.063	4.063	4.063	4.080	4.080	4.080
555	5.038	5.038	5.038	5.044	5.044	5.044
331	3.051	3.051	1.039	3.045	3.045	1.024
200	2.017	0.008	0.008	2.047	0.040	0.040
220	2.031	2.031	0.030	2.018	2.018	-0.011
11 $\bar{1}$	0.998	0.998	-1.013	0.978	0.978	-1.046
311	2.991	1.048	1.048	3.054	1.045	1.045
422	4.001	2.053	2.053	4.065	2.045	2.045
442	4.046	4.046	2.039	4.046	4.046	2.035
533	5.048	3.037	3.037	5.060	3.042	3.042
355	3.026	5.037	5.037	3.023	5.039	5.039
644	6.045	4.026	4.026	6.050	4.030	4.030
$\bar{1}11$	-1.014	0.998	0.998	-1.046	0.978	0.978
2 $\bar{2}0$	1.998	-1.998	0	2.000	-2.000	0
31 $\bar{1}$	3.002	1.011	-0.981	3.006	1.010	-0.990
3 $\bar{1}1$	3.000	-0.994	-0.994	3.007	-0.991	-0.991
2 $\bar{2}\bar{2}$	2.003	2.003	-1.987	2.002	2.002	-1.998
400	3.998	0.020	0.020	4.013	0.015	0.015
420	4.010	2.018	0.027	4.017	2.019	0.017
4 $\bar{2}0$	3.997	-1.990	0.006	4.000	-1.993	0.005

331	-2.991	2.996	1.001	-2.995	2.997	1.000
331	3.012	3.012	-0.981	3.013	3.013	-1.011
224	-1.986	2.005	4.001	-1.991	2.006	4.003
224	1.996	1.996	-3.993	-1.997	1.997	-3.997
333	-2.989	3.001	3.001	-2.993	3.001	3.001
115	1.023	1.023	5.000	1.017	1.017	5.021
115	-0.985	1.010	5.000	-0.990	1.009	5.005
115	0.991	0.991	-4.996	0.993	0.993	-5.001
440	4.019	4.019	0.019	4.020	4.020	0.014
440	3.993	-3.993	0	3.996	-3.996	0
531	5.019	3.021	1.025	5.027	3.024	1.019

FIGURE CAPTIONS

1. Interatomic potentials for Tungsten. Positions of the first, second and third nearest neighbors are indicated.
2. Core region for crowdion calculations. The crosses indicate perfect lattice sites while the circles correspond to the final relaxed positions. Altogether the core consists of 10 "interstitials" and 9 "vacancies".

Figure 1.

Figure 2.