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A faster way to relax interfaces in supercells

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Abstract

The usual way of minimizing the total energy of a planar boundary between two crystals by relaxing the atomic positions is inefficient, because it does not exploit the physical insight that forces are localized near the interfaces or surfaces. I introduce a simple change of variables, which leads to much faster and more accurate relaxation in such systems. In general the method is formulated for three-dimensional monoclinic supercells with sides (**a**, **b**, **c**), subject to periodic boundary conditions. If the crystals fill space the method exploits the stress tensor in the supercell to adjust its side **c**, where the boundary lies in the (**a**, **b**) plane, but the stress tensor is not required for a slab of finite thickness, which would be simulated by including a vacuum layer in the supercell. In either case the number of conjugate gradient steps required to relax the atomic positions does not increase with the thickness of the system. The power of this method is demonstrated by calculations on one-dimensional chains, both finite and infinite, using a pair potential to calculate the energy, forces and stresses.

1. Introduction

The general problem of finding the minimum energy configuration of the atoms around defects in crystals is relevant to the diverse fields of solid-state chemistry, materials science and geology. Mike Norgett's seminal contributions helped the field of atomistic simulation to take off in these disciplines, notably in his paper with Fletcher on fast matrix methods [1] and in his construction of the HADES code [2] which became the basis for a generation of scientists in which to devise sophisticated atomistic relaxation codes for defects. One such code, CHAOS, that included surfaces and interfaces, was developed and exploited extensively by Tasker and co-workers [3] and there were short steps to calculating phonon frequencies and free energies using the relaxed coordinates and applying the methods developed to problems in the earth sciences [4].

This paper deals with the common computational problem in materials science (see, for example, [5] for some case studies) of how to optimize the configuration of atoms and find the minimum total energy of planar boundaries with periodic boundary conditions. Periodic boundary conditions are a convenient tool in conjunction with first-principles or *ab initio*

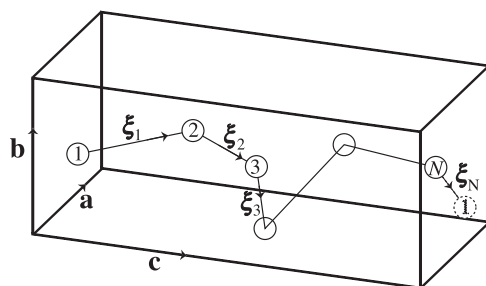


Figure 1. The supercell, its sides (\mathbf{a} , \mathbf{b} , \mathbf{c}) and the new variables ξ_i .

methods of calculating total energies, which nowadays can handle hundreds of atoms, e.g. [6], and will soon be dealing with thousands of atoms on a routine basis. My suggestion is that traditional methods of energy minimization, such as Newton–Raphson or conjugate gradients, although they work, are inefficient because they take no account of our prior knowledge that the relaxations are concentrated near the boundary. The straightforward change of variables introduced here, which mathematically represents a specific nonlinear preconditioning, leads to a dramatic reduction in computation time for such problems compared to a straightforward conjugate gradients method.

Let us consider an interface described by two juxtaposed crystalline slabs or *grains*, as we shall call them. The slabs are infinite in the (x, y) plane but of finite thickness in the z direction. Periodic boundary conditions on a cell containing the atoms (the *supercell*) are applied in all three directions. The lattice vectors (supercell vectors) in the (x, y) plane are \mathbf{a} and \mathbf{b} , and for interface calculations these will normally be held fixed, because we normally want to simulate the situation in which one of the grains is thick enough to impose constant \mathbf{a} and \mathbf{b} . The third lattice vector $\mathbf{c} = (c_x, c_y, c_z)$ may be treated as a variable. The supercell may include a layer of vacuum: in this case it includes two free surfaces besides the interface. Or it may be solid throughout, in which case the supercell contains two interfaces and its periodic extension represents a multilayered structure of alternating slabs. In the latter case one would like to construct the system so that these boundaries are equivalent, although this is not always crystallographically possible. Supercells may contain anything from tens to millions of atoms, depending on the physical system one is simulating and whether *ab initio* methods, in which electronic wavefunctions are obtained, or computationally much faster empirical potentials are used to describe the interatomic forces. I concentrate here on supercells because most techniques for energy minimization in solids, based on electronic structure calculations, work with them. A very similar idea for relaxing interfaces between semi-infinite crystals with just two-dimensional periodicity was developed and applied in the 1980s by Sutton and co-workers and is described in [7]. The present method differs in essence by exploiting the stress tensor, where appropriate.

The problem at hand is to relax the atomic positions so as to minimize the total energy $E(\{\mathbf{r}_i\}, \mathbf{c})$, where the index i labels the atom at $\mathbf{r}_i = (x_i, y_i, z_i)$. These relaxations, by whatever method they are performed, tend to require a large number of iterations and it is easy to see why. When the atomic positions are relaxed, e.g. by a conjugate gradients method, at constant \mathbf{c} , the first coordinates to be varied by the minimization algorithm will be those at or near the interface (or surface). Far from an interface or surface there will be no forces on the atoms, assuming they have been set up at their bulk equilibrium crystal positions. This is still true if there is a homogeneous strain in the crystal, in which case there is a homogeneous stress but no forces, because forces can be thought of as arising from a stress gradient. The relaxation

of the atoms near the interface will initiate a wave of displacement, travelling from iteration to iteration away from the interface, reflecting from the next interface or surface, and only gradually decaying to zero.

To enable relative bulk translations of the grains, either to change the excess volume or to allow a sliding displacement of the grains, it may be geometrically necessary to relax the cell side \mathbf{c} besides the atomic coordinates. This will be unnecessary if and only if there is a vacuum layer of sufficient width that interactions across the vacuum are negligible, because in that case the grains are free to make relative translations and relax all the stresses and forces within a fixed supercell. Note that our physically motivated wish to keep \mathbf{a} and \mathbf{b} constant implies that we are not interested in relaxing stress components σ_{xx} , σ_{xy} and σ_{yy} , but we shall want to relax the other three. Energy minimization with respect to the cell sides is made more efficient if we have access to these stress components. In this case the derivatives of the energy with respect to the components of \mathbf{c} are given by

$$\frac{1}{A} \left(\frac{\partial E}{\partial c_x}, \frac{\partial E}{\partial c_y}, \frac{\partial E}{\partial c_z} \right) = (\sigma_{zx}, \sigma_{zy}, \sigma_{zz}) \quad (1)$$

where A is the area of the supercell in the plane of the interface:

$$A = |\mathbf{a} \times \mathbf{b}|. \quad (2)$$

The derivatives in (1) are not at constant atomic positions $\{\mathbf{r}_i\}$ but at constant *fractional* positions (X_i, Y_i, Z_i) of the atoms in the supercell, where

$$\mathbf{r}_i = X_i \mathbf{a} + Y_i \mathbf{b} + Z_i \mathbf{c}. \quad (3)$$

This corresponds to the usual definition and calculation of stress, which refers to a homogeneous deformation of the specimen. We thus introduce a second complete set of variables for describing the system, namely $(\{X_i, Y_i, Z_i\}, \mathbf{c})$. There is no particular condition imposed on $(\mathbf{a}, \mathbf{b}, \mathbf{c})$, although in practice they are often orthonormal, which somewhat simplifies the equations. I emphasize that we are only considering a scenario in which \mathbf{a} and \mathbf{b} always remain constant. The explicit expressions for the fractional variables are

$$X_i = \mathbf{r}_i \cdot \mathbf{u} \quad Y_i = \mathbf{r}_i \cdot \mathbf{v} \quad Z_i = \mathbf{r}_i \cdot \mathbf{w}, \quad (4)$$

where $(\mathbf{u}, \mathbf{v}, \mathbf{w})$ are the dual lattice vectors:

$$\mathbf{u} = \frac{1}{\Omega} \mathbf{b} \times \mathbf{c} \quad \mathbf{v} = \frac{1}{\Omega} \mathbf{c} \times \mathbf{a} \quad \mathbf{w} = \frac{1}{\Omega} \mathbf{a} \times \mathbf{b} \quad (5)$$

and Ω is the volume of the supercell:

$$\Omega = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}). \quad (6)$$

It will be convenient to use a common vector notation for derivatives, so that, given any scalar f that depends on any vector \mathbf{k} , we define the Cartesian vector:

$$\frac{\partial f}{\partial \mathbf{k}} = \left(\frac{\partial f}{\partial k_x}, \frac{\partial f}{\partial k_y}, \frac{\partial f}{\partial k_z} \right). \quad (7)$$

The forces on the atoms are given by

$$\mathbf{F}_i = - \frac{\partial E}{\partial \mathbf{r}_i} \quad (8)$$

and the derivatives with respect to fractional coordinates are given by the non-Cartesian triplet:

$$\left(\frac{\partial E}{\partial X_i}, \frac{\partial E}{\partial Y_i}, \frac{\partial E}{\partial Z_i} \right) = \left(\frac{\partial E}{\partial \mathbf{r}_i} \cdot \mathbf{a}, \frac{\partial E}{\partial \mathbf{r}_i} \cdot \mathbf{b}, \frac{\partial E}{\partial \mathbf{r}_i} \cdot \mathbf{c} \right). \quad (9)$$

If we need to allow \mathbf{c} to vary, the derivative $\partial E/\partial \mathbf{c}$ can be used in the minimization algorithm on the same footing as the forces on atoms or as $(\partial E/\partial X_i, \partial E/\partial Y_i, \partial E/\partial Z_i)$ if we are working in relative coordinates. However, this does nothing to alleviate the convergence difficulty mentioned above, for the calculated stress will initially be due to the forces on atoms near the interface, whereas what one would *like* to happen is for the algorithm to leave untouched the interatomic spacings within the bulk of the grains, while relaxing the interlayer spacings near the interface (and surfaces if present). What current algorithms will actually do is to uniformly strain the system. Although this is the natural response conjugate to the stress, it introduces an erroneous strain in the grains that must be laboriously removed during subsequent iterations. This difficulty is overcome by the new procedure described below.

2. Change of variables

Suppose there are N atoms, labelled $i = 1-N$. The atoms are permanently labelled to start with in order of increasing z_i , but it should not matter if this order changes during the course of the iterations. If several atoms have the same value of z , they can be indexed in any order. Define

$$\xi_i = \mathbf{r}_{i+1} - \mathbf{r}_i, \quad \{1 \leq i < N\} \quad (10)$$

and

$$\xi_N = \mathbf{r}_1 + \mathbf{c} - \mathbf{r}_N. \quad (11)$$

These are the new variables (see figure 1). We have traded $N + 1$ variables for N , but there was a degree of freedom too many in the original set of variables, because the energy is invariant to translations. Thus we set $\mathbf{r}_1 = 0$ without loss of generality.

At first glance it looks as if ξ_N has a special status. However, this is not the case because of the periodic boundary conditions. Atom 1 has an image at $\mathbf{r}_1 + \mathbf{c}$ which we can think of as atom $N + 1$. The new variables describe all the independent interatomic distances in the infinite periodic system. Unlike the original set of variables, among which the supercell sides have a special status compared to the atomic positions, the new variables are all on an equal footing, which is advantageous for the relaxation algorithm.

The inverse transformation of variables is

$$\mathbf{r}_i = \mathbf{r}_1 + \sum_{j=1}^{i-1} \xi_j, \quad \{1 < i \leq N\} \quad (12)$$

$$\mathbf{c} = \sum_{j=1}^N \xi_j. \quad (13)$$

I emphasize that \mathbf{r}_1 is an arbitrary constant. Using these transformations, the variables ξ_i can be passed to a standard minimization routine, which within a line minimization will have to call a routine to calculate the energy $E(\{\xi_i\})$ and probably its derivatives $\partial E/\partial \xi_i$. That routine will first make the back transformation to $(\{\mathbf{r}_i\}, \mathbf{c})$ variables before calculating the energy and forces by established routines. These familiar forces will have to be converted to the conjugate forces $\partial E/\partial \xi_i$ before the line minimizer can use them, as described in the following section.

3. Conjugate forces

3.1. Derivation

It remains to obtain expressions for the forces conjugate to the ξ_i , or in other words the energy derivatives $\partial E/\partial \xi_i$. This is a matter of applying the chain rule of partial differentiation:

$$\frac{\partial E}{\partial \xi_i} = \sum_{j=2}^N \left(\frac{\partial E}{\partial X_j} \frac{\partial X_j}{\partial \xi_i} + \frac{\partial E}{\partial Y_j} \frac{\partial Y_j}{\partial \xi_i} + \frac{\partial E}{\partial Z_j} \frac{\partial Z_j}{\partial \xi_i} \right) + \frac{\partial E}{\partial \mathbf{c}}. \quad (14)$$

The terms for $j = 1$ are excluded on the assumption that (X_1, Y_1, Z_1) will be held equal to zero. We have also used $\partial \mathbf{c}/\partial \xi_i = 1$. The factors $\partial E/\partial X_j$, $\partial E/\partial Y_j$ and $\partial E/\partial Z_j$ are given in equation (9) in terms of the conventional forces. We now require expressions for the ξ_i derivatives: this is a straightforward exercise in applying the chain rule. Consider first the X_j derivative and write

$$\frac{\partial X_j}{\partial \xi_i} = \frac{\partial X_j}{\partial x_j} \frac{\partial x_j}{\partial \xi_i} + \frac{\partial X_j}{\partial y_j} \frac{\partial y_j}{\partial \xi_i} + \frac{\partial X_j}{\partial z_j} \frac{\partial z_j}{\partial \xi_i} + \frac{\partial X_j}{\partial \mathbf{c}} \Big|_{\{\mathbf{r}_k\}} \quad \{j > 1\} \quad (15)$$

in which on the right-hand side X_j is regarded as a function of $\{\mathbf{r}_k\}$ and \mathbf{c} . Using equation (4) we find

$$\frac{\partial X_j}{\partial x_j} = u_x \quad \frac{\partial X_j}{\partial y_j} = u_y \quad \frac{\partial X_j}{\partial z_j} = u_z. \quad (16)$$

Similar equations hold for the position derivatives of Y_j and Z_j . From (12) we find

$$\frac{\partial x_j}{\partial \xi_i} = (1, 0, 0) \quad \frac{\partial y_j}{\partial \xi_i} = (0, 1, 0) \quad \frac{\partial z_j}{\partial \xi_i} = (0, 0, 1) \quad \{i < j\} \quad (17)$$

$$\frac{\partial x_j}{\partial \xi_i} = \frac{\partial y_j}{\partial \xi_i} = \frac{\partial z_j}{\partial \xi_i} = 0 \quad \{i \geq j\}. \quad (18)$$

The \mathbf{c} derivatives are given, after a little vector calculus, by

$$\frac{\partial X_j}{\partial \mathbf{c}} \Big|_{\{\mathbf{r}_k\}} = -Z_j \mathbf{u} \quad \frac{\partial Y_j}{\partial \mathbf{c}} \Big|_{\{\mathbf{r}_k\}} = -Z_j \mathbf{v} \quad \frac{\partial Z_j}{\partial \mathbf{c}} \Big|_{\{\mathbf{r}_k\}} = -Z_j \mathbf{w}. \quad (19)$$

After substituting these derivatives into (14) we find in terms of the usual variables

$$\begin{aligned} \frac{\partial E}{\partial \xi_i} &= \sum_{j=1}^N Z_j \{(\mathbf{F}_j \cdot \mathbf{a})\mathbf{u} + (\mathbf{F}_j \cdot \mathbf{b})\mathbf{v} + (\mathbf{F}_j \cdot \mathbf{c})\mathbf{w}\} \\ &\quad - \sum_{j=i+1}^N \{(\mathbf{F}_j \cdot \mathbf{a})\mathbf{u} + (\mathbf{F}_j \cdot \mathbf{b})\mathbf{v} + (\mathbf{F}_j \cdot \mathbf{c})\mathbf{w}\} + (\sigma_{zx}, \sigma_{zy}, \sigma_{zz})A \\ &= \sum_{j=1}^N Z_j \mathbf{F}_j - \sum_{j=i+1}^N \mathbf{F}_j + (\sigma_{zx}, \sigma_{zy}, \sigma_{zz})A. \end{aligned} \quad (20)$$

For $i = N$ the second summation should be omitted. Notice that I have reinstated the $j = 1$ term in the first summation. This is allowed trivially by our assumption that $Z_1 = 0$. However, it is not restricted to that assumption. For suppose we displace the supercell, such that a constant term is added to all the fractional coordinates, including Z_1 . Because the forces must sum to zero, this makes no difference to the summation in (20). Equation (20) is the central result we need, expressing the new energy derivatives in terms of the familiar forces on atoms and the stress in the supercell.

3.2. Comment on the case of a vacuum layer

Supercell calculations are often designed to include a vacuum layer, either to simulate surfaces deliberately or to avoid an awkward second boundary that might, for example, complicate a study of the energy of a single boundary. It is natural to label the atoms 1– N across the slab, in which case the absence of interactions across the vacuum implies that

$$\frac{\partial E}{\partial \xi_N} = 0. \quad (21)$$

The three $\sigma_{z\alpha}$ stress components in this situation are directly expressible in terms of forces on the atoms (although the other three are not) and there is no need to relax the shape of the supercell by changing \mathbf{c} . It is easy to show that in this case, with the natural numbering of atoms,

$$(\sigma_{zx}, \sigma_{zy}, \sigma_{zz}) = -\frac{1}{A} \sum_{j=1}^N Z_j \mathbf{F}_j \quad (22)$$

so that equation (20) reduces to

$$\frac{\partial E}{\partial \xi_i} = -\sum_{j=i+1}^N \mathbf{F}_j \quad \{i < N\}. \quad (23)$$

Equation (23), which represents a linear preconditioning, is the appropriate formula to use for simulating bicrystals, or simply if a slab of single crystal is set up to simulate free surfaces without any internal boundary. It has a simple interpretation. The summation on the right-hand side represents the total force on the block of atoms to the right of the interplanar spacing described by ξ_i . To relax the conjugate force, that block will move rigidly, without disturbing its crystal structure, which is physically what one would want.

4. Test calculations

As a preliminary to a full implementation of this approach I have made some test calculations for a simple one-dimensional model, consisting of a chain of N atoms interacting through an arbitrarily chosen 4–8 potential of the Lennard-Jones form:

$$V(r) = 4\epsilon((\sigma/r)^8 - (\sigma/r)^4), \quad (24)$$

with a cut-off at $r = 3\sigma$. The chain was set up at its bulk equilibrium interatomic spacing, $a_0 = 1.172461\sigma$. Two very different situations were considered. In the situation I will call the ‘free chain’ the N atoms were terminated by a ‘vacuum layer’ of the same length Na_0 as the chain, so the repeat length of the supercell was chosen to be $L = 2Na_0$. For practical purpose this is equivalent to a free finite chain and we want to relax its ‘surfaces’. In the second situation, the ‘infinite chain’, the chain was periodically repeated in a continuous fashion by choosing a repeat length of $L = Na_0$, but to provide an ‘interface’ atom N was shifted back along the chain by 10% of the interatomic spacing. For the infinite chain, besides the fractional atomic positions of atoms 2– N , the stress is relaxed by including the repeat length L as a variable in the energy minimization.

The ‘old’ relaxation procedure, for which I report results in table 1, uses standard Fletcher–Reeves conjugate gradients, as described in [8]. In this 1D case the variables are $(\{Z_i\}, c_z; 1 < i \leq N)$ for the infinite chain. The convergence criterion I have used throughout is to reduce the maximum force on any atom to below $10^{-4}\epsilon/\sigma$ and the fractional energy change per iteration to 10^{-7} . The ‘new’ relaxation procedure, results of which are also

Table 1. Number of conjugate gradient iterations required for convergence using ‘old’ and ‘new’ algorithms for two systems. ‘Free chain’ is a finite chain of length N atoms, which start equally spaced. ‘ ∞ chain’ is a periodically repeated chain of N atoms, of which 1 is initially displaced by 10% of the nearest-neighbour distance.

N	Free chain		∞ chain	
	Old	New	Old	New
10	9	2	41	8
20	16	2	29	8
30	21	2	37	8
40	26	2	46	8
50	24	2	56	8
60	29	2	66	8
70	35	2	76	8
80	39	2	72	8
90	44	2	72	8
100	49	2	72	8
120	59	2	72	8
140	65	2	72	8
160	65	2	72	8

in table 1, uses exactly the same minimization algorithm and convergence criterion on the maximum force on an atom and energy change, but it iterates on directions in the space of the variables ($\{\xi_{iz}\}; 1 \leq i \leq N$). For the free chain the variable Z_1 was included in the ‘old’ relaxation procedure, which approximately halved the number of iterations required because the symmetry of the system is thereby preserved.

The supercell length L for the free chain plays no part in the relaxation. It would do so in the old relaxation procedure if we used the stress to change the length of the supercell as we do in the infinite chain.

5. Results and discussion

The results in table 1 illustrate the very rapid convergence of the preconditioned algorithm, which requires 2 line searches for the free chain and 8 for the infinite chain, independent of chain length. This is as expected, since the algorithm only adjusts the interatomic spacings very near the surfaces of the chain or near the defect, respectively. On the other hand the standard conjugate gradient method, starting with a line search in the direction of steepest descent, requires a number of iterations that scale roughly linearly with the number of atoms until it reaches a plateau of 72 iterations for the infinite chain or 65 for the free chain. What is happening here was confirmed by watching a movie of the relaxation in which the atoms were coloured according to the forces on them. A soliton-like wave of disturbance propagates from the defect or surface into the chain, at a rate of one atom per iteration, gradually decaying in amplitude and spreading as it does so. The maximum force within this disturbance must travel through about $N_c = 70 \pm 5$ atoms before its amplitude has decayed sufficiently to satisfy the present maximum force convergence criterion. For the infinite chain with more than this number of atoms, the ‘old’ method does not need to adjust atomic positions further from the defect than N_c atoms, so the number of iterations becomes constant for $N > N_c$.

For the free chain, there are two surfaces from which the ‘old’ method causes equivalent disturbances to propagate and convergence occurs roughly when they meet in the centre of the chain or when they have travelled N_c atoms, whichever happens first. For $N > 2N_c$ the

relaxation therefore terminates in about $2N_c$ iterations. Note that this does not imply that the computation time becomes independent of N , because not only do all the forces have to be calculated at every iteration, but also the line search associated with each iteration itself requires more iterations as the number of variables increases. In large systems the new algorithm simply never disturbs the regions so far from the interfaces as the old one does and therefore involves fewer variables in the line searches.

6. Summary and conclusions

I have introduced an algorithm for relaxing surfaces and interfaces comprising N atoms in a supercell, with periodic boundary conditions. It is based on using N interatomic vectors ξ_i , ($1 \leq i \leq N$), as variables and requires much fewer conjugate gradient (CG) relaxations compared to applying the CG method directly to the individual atomic positions and (where appropriate) supercell sides. Two typical simulation situations can be distinguished. In the first the supercell (**a**, **b**, **c**) describes non-interacting slabs in the (**a**, **b**) plane, separated by vacuum layers. In the second it describes a space-filling multilayer of slabs. In the second situation, three components of the stress tensor, namely $\sigma_{z\alpha}$, ($\alpha = x, y, z$), are required to completely relax the energy of a supercell at fixed (**a**, **b**). In the conventional approach they would be used to relax side **c** of the supercell, but in the new approach they enter the expression (20) for the forces conjugate to the ξ_i , and **c** is slaved to these new variables. In both situations the new algorithm converges within a constant number of CG steps that does not increase with the thickness of the slabs. The conventional approach requires a number of CG steps that scales linearly with the thickness of the slabs up to a maximum that depends on the maximum force allowed when convergence is deemed to have been reached. Simple one-dimensional calculations have verified the effectiveness of the method and suggest that it can save orders of magnitude in computer time. This is likely to be of particular value in large scale *ab initio* calculations.

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