

Department of Physics, Chemistry and Biology

Master's Thesis

**First-principle studies of Sc/Cr multilayers for
x-ray mirrors applications**

Jonatan Abramsson

LiTH-IFM-1907/08-SE

Department of Physics, Chemistry and Biology
Linköpings universitet, SE-581 83 Linköping, Sweden

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Jonatan Abramsson

Adviser: **Arkady Mikhaylushkin**
IFM
Till Burkert
IFM

Examiner: **Igor Abrikosov**
IFM

Linköping, 25 February, 2008

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Titel Title	Studier av Sc/Cr multilager, vars tillämpning är röntgen spegling First-principle studies of Sc/Cr multilayers for x-ray mirrors applications	
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Sammanfattning Abstract <p>In order to produce x-ray mirrors the Thin Film Physics group at IFM grows Cr/Sc multilayers, with a typical thickness of the individual layers in the range 5-20 Å, and with as many periods as possible (a few hundred). The quality of the multilayer interfaces is crucial for their performance as mirrors. For thick layers poly-crystalline multilayers form with an interface quality that is too poor for the use as x-ray mirrors. For thinner layers, however, amorphous layers are formed with a much better quality of the interface.</p> <p>The goal of this project was to understand the formation of amorphous multilayers. Unfortunately it is impossible with the present day's theoretical tools to determine the structure of amorph interfaces. It is also impossible to calculate the interface structure for elements with large mismatch in size.</p> <p>So we have to construct interface models that are both simple and based on physical arguments.</p>		
Nyckelord Sc, Cr, interface, x-ray mirror Keywords		

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Abstract

In order to produce x-ray mirrors the Thin Film Physics group at IFM grows Cr/Sc multilayers, with a typical thickness of the individual layers in the range 5-20 Å, and with as many periods as possible (a few hundred). The quality of the multilayer interfaces is crucial for their performance as mirrors. For thick layers poly-crystalline multilayers form with an interface quality that is too poor for the use as x-ray mirrors. For thinner layers, however, amorphous layers are formed with a much better quality of the interface.

The goal of this project was to understand the formation of amorphous multilayers. Unfortunately it is impossible with the present day's theoretical tools to determine the structure of amorph interfaces. It is also impossible to calculate the interface structure for elements with large mismatch in size.

So we have to construct interface models that are both simple and based on physical arguments.

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Chapter 1

Introduction

1.1 Background

1.1.1 X-ray mirrors

The development of multilayer mirrors is necessary for the development of telescopes for deep space astronomy[1], x-ray microanalysis[2] and the optics in free-electron lasers[3]. Multilayer ultra thin mirrors are also necessary for the development of compact soft x-ray microscopes[4], soft x-ray polarimetry[5] and the next generation of extreme ultraviolet lithography[6].

For all instruments that involve soft x-ray the main factor limiting the performance is the optical elements[7]. If we can build optical elements with much higher spectral resolution, stability and reflectivity we will develop many x-ray fields. This can only be done if we have multilayer mirrors with smooth surfaces and with a layer width that can be special made for the wavelength used[7].

1.2 Thesis outline

1. In chapter 2 I discuss the fundamental theory with all approximations and equations.
2. In chapter 3 I discuss the program VASP that I have been using.
3. In chapter 4 I discuss what I have done and why. I also discuss all my results and what they mean.
4. In chapter 5 I give a short summary of what my results mean.
5. In chapter 6 I talk a bit about what can be done in the future.

1.3 Project Aims

The primary goal of this work was to study interface energy in Sc/Cr system as a function of the multilayer thickness. In order to do that we have to investigate the optimal positions for Sc and Cr atoms in a Sc/Cr multilayer mirror for wavelengths in the X-ray spectra. I hope to find suitable structures that does not cost a huge amount of energy for the experimentalists to build. But probably I can at least help them to understand their results so they can do a more directed search for an optimal layer structure.

1.4 Summary of the Computational Process

A short summary of the process to receive the results.

1. The first bulk energy is given by calculations of pure Sc and Pure Cr.
2. When I calculated the total energies I first set up my parameters so that I allowed the atoms to move a bit in relation to each other while I minimized the energy.
3. After I found the optimal positions for the atoms in my crystal I calculated the total energy.
4. When I got the bulk energy and the total energy I calculated the interface energy by equation 1.1.

$$E_{total} = E_{interface} + E_{bulk} \quad (1.1)$$

Chapter 2

Theory

2.1 Density function theory

I have used a method called Density function theory (DFT). DFT is a theory commonly used for calculation on crystals with ground state energy.

2.1.1 First-principle calculations

The calculations in DFT are so called First-principle calculations. They start with the laws of Quantum mechanics. First-principle calculations can be approximated using non-relativistic treatment, so we use the Schrödinger equation instead of the Dirac equation. For this project time is not important so the equation that we use is the time independent Schrödinger equation:

$$\hat{H}\Psi = E\Psi \quad (2.1)$$

with a wavefunction that looks like this:

$$\Psi = \Psi(R_1, R_2, \dots, R_n, r_1, r_2, \dots, r_m) \quad (2.2)$$

where the R is the positions of the nucleus, r is the positions of the electrons, n is the number of nucleus and m the number of electrons.

The Hamiltonian looks like this:

$$\hat{H} = -\frac{\hbar^2}{2m_e} \sum_i \nabla_i^2 + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_i - r_j|} - \frac{\hbar^2}{2} \sum_k \frac{\nabla_k^2}{M_k} + \frac{1}{2} \sum_{k \neq l} \frac{Z_k Z_l}{|R_k - R_l|} - \sum_{i,k} \frac{e Z_k}{|r_i - R_k|} \quad (2.3)$$

which can be written like this

$$\hat{H} = \hat{T}_e + \hat{V}_{ee} + \hat{T}_n + \hat{V}_{nn} + \hat{V}_{en} \quad (2.4)$$

T is the kinetic energy, V is the potential energy for electron-electron, electron-nuclei and nuclei-nuclei interaction.

Solving the Schrödinger equation is impossible for systems with more than 2 particles. Therefore we are forced to make some more approximations.

2.1.2 The Born-Oppenheimer Approximation

The first approximation that we do is to say that the nucleus is still relative the other nuclei. That makes the potential energy of the nuclei constant and the kinetic energy of the nuclei zero.

$$\hat{T}_n = 0 \quad (2.5)$$

and

$$\hat{V}_{nn} = \text{constant} \quad (2.6)$$

This approximation is justified by the fact that the nucleus weighs about 2000 times more than the electron which makes it more inert.

2.1.3 The Hohenberg and Kohn theorems

The density function theory is a quite clever theory. The general thought of it is to replace all the electrons' degrees of freedom with an electron density. 3m degrees of freedom is then replaced by 3 degrees of freedom. Hohenberg and Kohn did this by formulating two theorems on this matter[8].

- The local external potential, $V_{ext}(r)$ is within a constant, determined by the electron density of the ground-state $n(r)$.
- The total energy function, $E[n(r)]$ is minimized for the correct electron ground-state density, $n(r)$ with a given local external potential, $V_{ext}(r)$.

With these theorems Hohenberg and Kohn reduced the many-body problem with many one-body problems. But one problem remains to solve. How can we calculate the total energy with all these electron-electron interactions?

2.1.4 The Kohn and Sham equations

One year after Hohenberg and Kohn presented their theorems Kohn and Sham presented a way to solve the electron-electron interaction problem. By replacing all the interacting electrons with non-interacting quasi particles and making these quasi particles yield exactly the same electron density $n(r)$ they made our problem possible to solve[9].

$$\left[-\frac{\hbar^2}{2m_e} \nabla^2 + V_{eff}(r) \right] \psi_i(r) = \epsilon_i \psi_i(r) \quad (2.7)$$

$\psi_i(r)$ is the single particle orbitals and $V_{eff}(r)$ is the potential that our quasi-particles act in and can be expressed like[10]:

$$V_{eff}(r) = V_{ext} + \int \frac{n(r')}{|r-r'|} dr' + \frac{\delta E_{xc}[n(r)]}{\delta n(r)} \quad (2.8)$$

$$n(r) = \sum_{i=1}^N |\psi_i(r)|^2 \quad (2.9)$$

The problem is now down to the exchange-correlation energy, $E_{[n(r)]}$ part.

Equation (2.7), (2.8) and (2.9) are the Kohn-Sham equations and they can be solved by an iterate method.

2.1.5 The Local Density Approximation

One idea for solving the exchange-correlation energy problem was first suggested by Kohn and Sham[9] in 1965 as the Local density approximation, (LDA). Kohn and Sham assumed that many crystal materials could be described as homogenous electron gases. With a homogenous electron gas the effect of correlation and exchange is local. Therefore the exchange-correlation function looks like this:

$$E_{xc}^{LDA}[n(\mathbf{r})] = \int \epsilon_{xc}[n(\mathbf{r})]n(\mathbf{r})d\mathbf{r} \quad (2.10)$$

where ϵ_{xc} is the exchange-correlation energy density per particle in a uniform electron gas and n is the density of that electron gas.

LDA often works best for systems with an electron structure close to a homogenous gas and worst for systems like a single atom[11]. Systems that are not optimal for LDA usually only underestimate the lattice parameters of the equilibrium point with 1-3 % and the exchange-correlation energy by 7 %[12].

2.1.6 The Generalized Gradient Approximation

Another approximation that we can use is the Generalized Gradient Approximation (GGA). GGA is a more complex approximation than LDA and often gives a better result¹. In the GGA the form of the exchange-correlation energy from LDA is improved with a local density gradient. The exchange-correlation energy then looks like equation (2.11)[13].

$$E_{xc}^{GGA}[n(\mathbf{r})] = \int f[n(\mathbf{r}), \nabla n(\mathbf{r})]n(\mathbf{r})d\mathbf{r} \quad (2.11)$$

There are several different GGA functions with different strength and weaknesses, because there is not a unique way to add gradients to a function. Whether it is better to use LDA or some GGA depends on the type of calculation. I have used GGA for the calculations in this project.

¹A result closer to data given by studies of real matter.

2.1.7 Limitations of DFT

In the DFT method we put all our approximations in the LDA or the GGA part. If the LDA or the GGA is not a good approximation the DFT is a less good method to use. If the LDA or GGA is a good approximation it is easy to calculate the ground state and get the systems Hamiltonian. Once we have the Hamiltonian for the system we can calculate all excited states for example temperature over zero or core-level shifts. That is why the DFT method is so popular.

Another problem is that errors move through the system. An approximation in a real calculation results in a ground state that is not quite correct, which give us a Hamiltonian with an error. This makes our calculated excited states differ from the actual excited state. As when you calculate pure iron (Fe) with LDA the result tells us that Iron has in its ground state a nonmagnetic fcc-structure and not a ferromagnetic bcc-structure, as we all know that it has[12, 14, 15].

To reveal if GGA or LDA is a good approximation, I calculated the energies for pure Cr and pure Sc using GGA and LDA. I found when comparing to known values that the Generalized Gradient Approximation well suited the calculations in our project.

Chapter 3

Calculation Methods

3.1 The Vienna ab initio simulation package, VASP

In this project I have done electronic structure calculations using the projector augmented wave method, [16], PAW. VASP is the program that I have used for my calculations. The PAW method is included in VASP [17]. The wave function in the PAW method is a superposition of plane waves and expansions into atomic pseudo orbitals in just one basis set [18]. The plane waves are good for describing the wavefunction far away from the nucleus and the expansion into atomic orbitals are good for describing parts near the atomic nucleus.

When we use computers to efficiently solve the Kohn-Sham equations (2.7), (2.8) and (2.9) we have to use the PAW method to expand the wave functions in a basis set. This can be done without a great loss of generality.

The method is based on a linear transformation that maps the set of all electron valence functions ψ_i to the smooth function ψ_j [18].

$$|\psi_i\rangle = \sum_j c_j |\psi_j\rangle \quad (3.1)$$

If equation (3.1) is inserted in equation (2.7) we get:

$$\sum_j c_j \hat{H}_{eff} |\psi_j\rangle = \epsilon_i \sum_j c_j |\psi_j\rangle \quad (3.2)$$

If we then multiply equation (3.2) with $\langle\phi_k|$ from the left we get:

$$\sum_j c_j \langle\psi_k| \hat{H}_{eff} |\psi_j\rangle = \epsilon_i \sum_j c_j \langle\psi_k| \psi_j\rangle \quad (3.3)$$

Where the matrix of the Hamiltonian is:

$$H_{kj} = \langle\psi_k| \hat{H}_{eff} |\psi_j\rangle \quad (3.4)$$

And equation (3.5) is the overlap integral of the different basis functions

$$O_{kj} = \langle \psi_k | \psi_j \rangle \quad (3.5)$$

Then it is possible to see that equation (3.3) can be written as

$$\sum_j c_j (H_{kj} - \epsilon_i O_{kj}) = 0 \quad \forall k \quad (3.6)$$

This set of linear algebraic equations has of course only non-trivial solutions if:

$$\det [H_{kj} - \epsilon_i O_{kj}] = 0 \quad (3.7)$$

Solving this set of equations gives us the eigenvalues ϵ_i and the coefficients c_j . These eigenvalues, ϵ_i of the Schrödinger equation give the electronic band structure[18]. When we have the band structure it is possible to see if a material is an insulator, semiconductor or metal. A semiconductor has a bandgap between 0 and 4 eV, the insulator over 4 eV and a metal 0 eV.

We have to know that the eigenvalues calculated in equation (3.6) do not correspond to a single electron system. The Kohn-Sham orbitals do not fit the single electron state very well and that results in DFT underestimating the bandgap in a semiconductor by a few eV[18].

Chapter 4

Results and discussion

What is well known is that Sc has its lowest energy in hcp structure. When I was calculating the energies for pure Sc I found that bcc structure had the highest potential energy. In Majkova's article[19] we can see that the length of a Sc - Cr multilayer increases just 2.4 % when heating the multilayer and that it does not affect the reflectivity much. This increase in length could be a result of a structural change in the Sc and/or Cr layers. Conclusively the structure should not affect us that much.

When calculating the equilibrium states for pure Sc and pure Cr I found that Sc is much bigger than Cr, about 25 % bigger. Sc as bcc has a lattice constant of 3.65 Å and Cr in bcc structure has a lattice constant of 2.91 Å. There is a problem with calculating the surface structure of elements with a big mismatch in size because it is hard to find positions for the atoms that do not generate big forces.

Then I calculated the energies for pure Sc and pure Cr using the equilibrium states, which gave me my bulk energies for pure Sc and pure Cr.

After that I calculated the total energy of my layer structures. These layer structures are discussed in the sections below.

4.1 Interfaces in Sc/Cr multilayers

I have calculated the energy in the interface between layers of Sc and Cr and I have tried to minimize this energy. To do this I have checked some different structures. I chose to test only three structures because time and computer power was a limitation. By a lot of thinking and a rotating paper method (see section 4.2.3) I found that one of these three structures should have the lowest energy.

- bcc-Sc on bcc-Cr rotated 45 degrees
- fcc-Sc on bcc-Cr rotated 45 degrees
- bcc-Sc on bcc-Cr rotated 18,4 degrees

VASP is a program that calculates the total potential energy in a chosen system we can choose this system to be just one Sc bulk, one Cr bulk and one interface.

It is easy to realize that the potential energy in the multilayer has to be a sum of the energy in the bulk times the number of bulks plus the energy in the interface times the number of interfaces.

$$E_{total} = E_{interface} + E_{bulk} \quad (4.1)$$

$$E_{bulk} = n * E_{bulk}(Sc) + m * E_{bulk}(Cr) \quad (4.2)$$

n is the number of Sc atoms and m the number of Cr atoms in the crystal. By equation (4.1) and (4.2) we got our interface energy.

$$E_{interface} = E_{total} - n * E_{bulk}(Sc) - m * E_{bulk}(Cr) \quad (4.3)$$

4.2 Structural models for interfaces

4.2.1 bcc-Sc on bcc-Cr rotated 45 degrees setup

I started by entering atom-positions of Cr - bcc on top of Sc - bcc, rotated 45 degrees in VASP. The distance miss-match for Sc (000) - Sc (100) divided to Cr (000) - Cr (110) is about 11%, that is 5,5% per atom. This miss-match will bring some forces in the crystal but it should probably be OK. Because of the big difference in lattice parameter I was able to put two Cr cells on one Sc cell. And because VASP require periodic boundary conditions during the calculation there have to be an extra pair of Cr on top (as you can see in figure 4.1 and 4.3) so that the crystal could duplicate in z - direction. Actually it is more like two whole and two half Cr cells on top of one cell Sc, though I will still call it 1Sc1Cr.

After I calculated the total energy of 1Sc1Cr I then calculated the total energy of 2Sc2Cr. The 2Sc2Cr structure is the same as 1Sc1Cr but with one more Sc cell on top of the Sc layer and two more Cr cells on top of the Cr cell layer. I present this model in figure 4.1 by adding Sc atom layer 1 and 2 to the original Sc atom layer 3 and 4. I also calculated the total energy for 4Sc4Cr and 8Sc8Cr.

In figure 4.1 we see how layers of Cr and Sc are put together from a y - z view. Figure 4.2 shows how Sc and Cr fit together from an x - y view. In figure 4.1 and 4.2 the circles represent Sc atoms and the dots represent Cr atoms. Atom layer two in figure 4.1 is the body centered atoms to the atoms in layer one. With the same relation between layer three and four. The atoms in layer two and four are a half atomic distance down in x - direction. This is represented with smaller rings in layer two and four. On top of Sc layer one to four there is three layers of Cr. Cr has smaller distances and there goes approximately two Cr unit cells on one Sc unit cell as we can see in figure 4.2 therefore we must put two atoms in layer 5 per atom in layer 4. We can see in figure 4.2 that the Cr atoms in the layer on top of the last Sc layer is not right above the Sc atoms and they differ in x - axis. That is why some Cr atoms look smaller in figure 4.1 than the other Cr atoms. They are positioned like some Sc atoms a bit down in x - direction. The atoms in layer six and layer five are forming bcc cells, with the atoms in layer six as the body

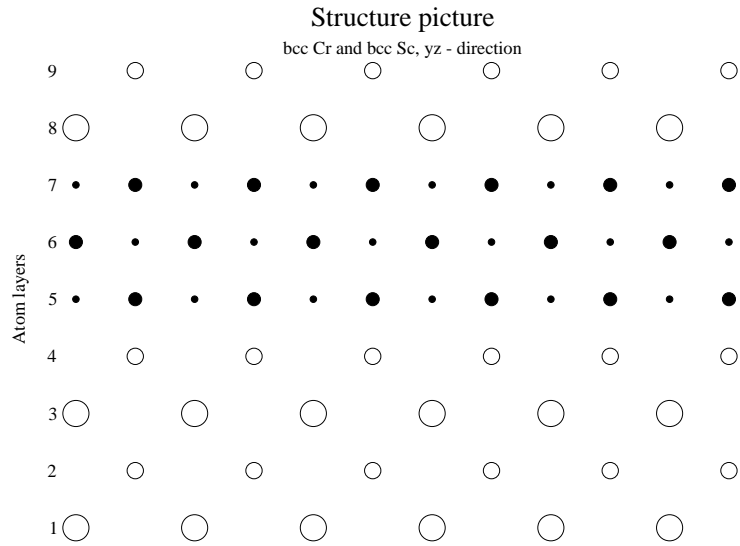


Figure 4.1. Layer picture, bcc structure, 2Sc - 1.5Cr - 1Sc

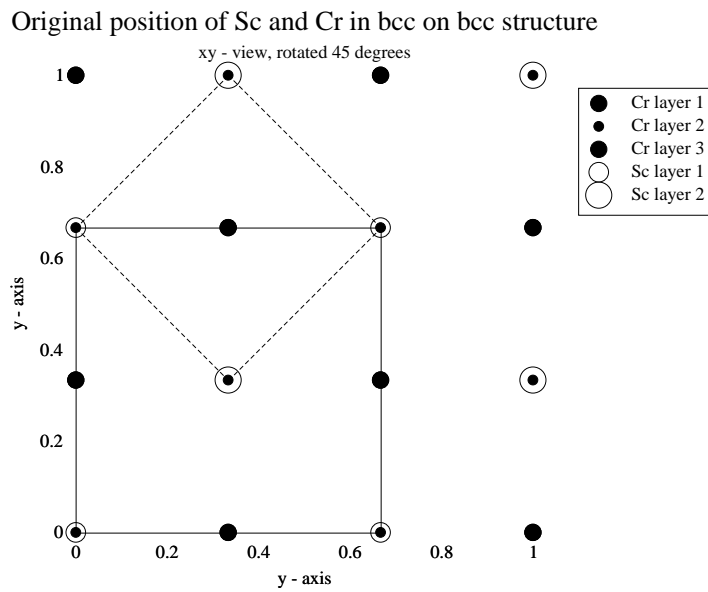


Figure 4.2. Layer picture, bcc structure, (x,y) - direction

centered atoms. Layer seven is an extra layer of Cr to make it possible to put Sc on top of the Cr layers which we want to do when we build multilayers.

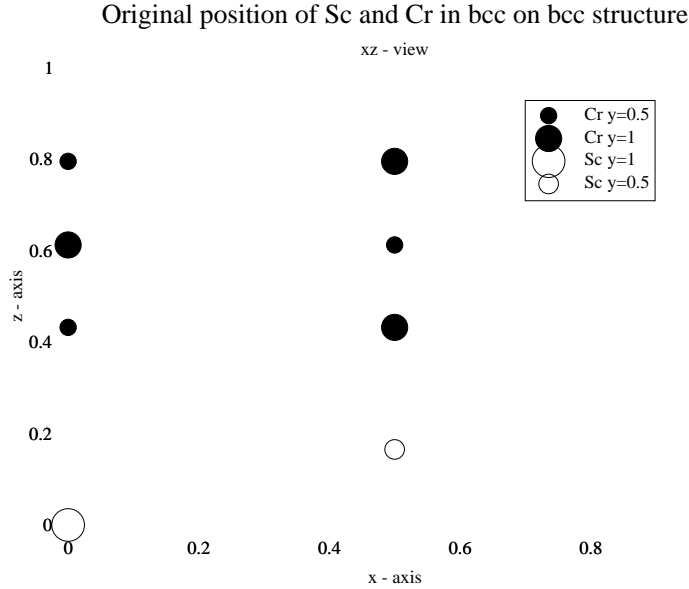


Figure 4.3. Layer picture, bcc structure, 1Sc cell - 1.5Cr cell

I have used the smallest part of the crystal, which if repeated generates the whole crystal to save computer power. When I was calculating 1Sc1Cr I used the structure in figure 4.3.

4.2.2 fcc-Sc on bcc-Cr rotated 45 degrees setup

The difference between fcc-Sc on bcc-Cr and bcc-Sc on bcc-Cr is not that big. Because an fcc-structure cell can be seen as two bcc-structure cells rotated 45 degrees. The only difference is a factor $\frac{1}{\sqrt{2}}$ in z-direction. So I use the same setup as when I calculated bcc-Sc on bcc-Cr but with $\sqrt{2}$ times longer distances in z-direction. Then I calculated the energies for 1Sc1Cr, 2Sc-2Cr and 4Sc-4Cr.

4.2.3 bcc-Sc on bcc-Cr rotated 18.4 degrees setup

The idea to rotate the Cr layers 18.4 degrees compared to the Sc layers came from my so called Rotated Paper Method, RPM. RPM is a quite simple and fast method to see which crystal structures could generate a low interface energy. The trick is to print or draw a one cell thick layer, of the materials that you want to put together, on two separate papers in a relevant proportion according to each other. The materials have to be printed in all the structures that they may have, in their

lowest energy and in a direction that you want to use. To generate a possible structure from RPM you lay one paper of one material on top of a paper of the other material and try to find positions of the atoms that may cause low structural forces as I mentioned at the beginning of section 4.2.1. When you think you have found atoms that do not shift that much in distance you take these atoms as a starting pattern and generate your primitive cell. Then you take your primitive cell and take a good look at it to see if there are any atoms in it that could generate a high potential energy. If there are atoms generating high potential energy in your primitive cell you have to remove one of these atoms or find another primitive cell. Keep in mind that you in VASP can let your atoms move a bit to find a better structure.

I found by RPM a primitive cell that could suite our purpose. When rotating my bcc-Sc 18.4 degrees compared to my bcc-Cr sheet I found a distance miss match for Sc (000) - Sc (120) divided to Cr (000) - Cr (220) is about 0.84 %, that is almost nothing per atom compared to the 45° shift. The atoms inside my primitive cell seemed to fit well in a starting-structure for VASP to calculate. This primitive cell setup is shown in figure 4.4.

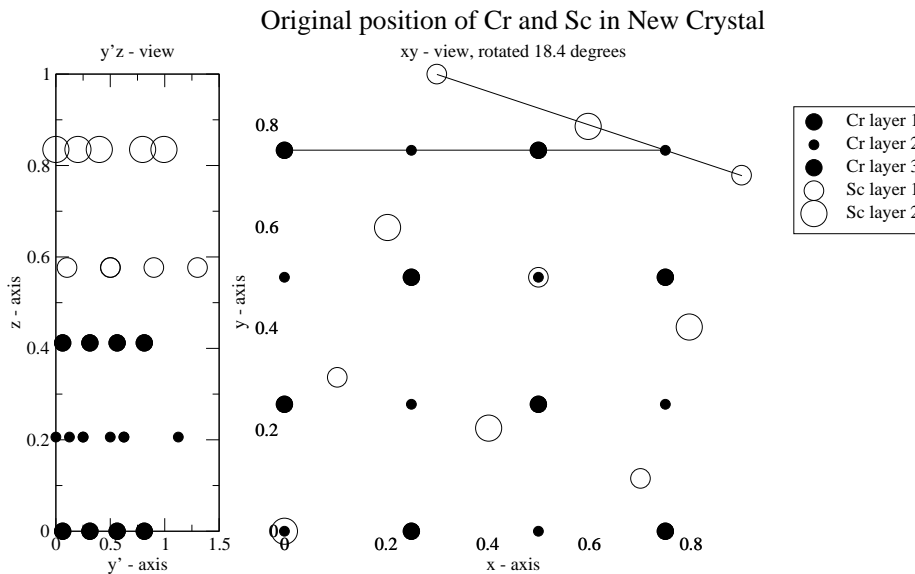


Figure 4.4. Layer picture, New crystal structure, (x,y) - direction and (y',z) - direction

Figure 4.4 shows the setup positions for Sc and Cr a crystal that I call the New crystal. To the left is the crystal described from $z-y'$ view, where $y' = \sqrt{x^2 + y^2}$. Sc is represented like in figure 4.1, 4.2 and 4.3 by circles and Cr by dots. The right part of the figure shows the crystal from the $x-y$ view. The two lines in the right part of the figure shows the 18.4° shift between Sc and Cr.

4.3 Relaxed structures

In order to optimize atomic positions for the structural models suggested above, I carried out self-consistent DFT calculations for Sc/Cr multi-layers in which I relaxed the system so the forces between the atoms could be minimized. This made each atom move to a position with a lower potential energy.

4.3.1 45 degree shift

In figure 4.5 I show interlayer distances versus layer number.

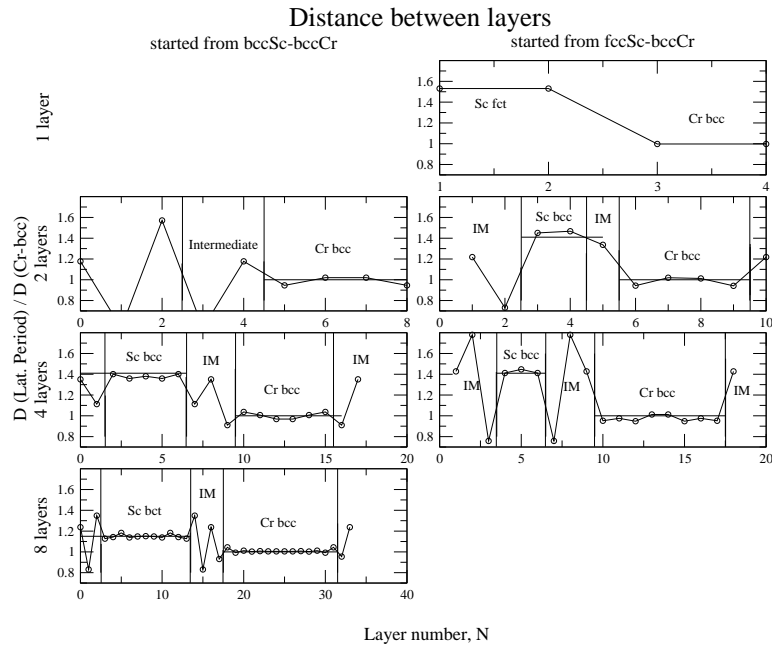


Figure 4.5. Layer distance

There are two columns in figure 4.5, the left one is based from bccSc-bccCr and the right one is based from fccSc-bccCr. On the y-axis we got the interlayer distance, which coordinates are normalized to the half bcc lattice constant in the atomic distances for Cr.

The vertical lines in figure 4.5 separate areas with Cr-Cr boundary with Sc-Cr and Sc-Cr with Sc-Sc. The areas called IM is the intermediate areas where the Cr atoms are interacting with the Sc atoms more than in other areas. The horizontal lines are the average inter atomic distances. The Cr-bcc line is of course equal to 1. Sc-bcc line is $=\sqrt{2}$ because of the 45 degree rotation. If the inter atomic distance is bigger than $\sqrt{2}$ we call the structure fct and if the interatomic distance

is less than $\sqrt{2}$ we call it bct. Bcc, fcc, fct and bct are in fact the same structure but with different distances and different unit cells [20].

In figure 4.5 we see that the calculations that I start from bccSc - bccCr go to bctSc - bccCr for eight layers. But for four and two layers they stay bccSc - bccCr. The calculations based on fccSc - bccCr go to a bccSc - bccCr structure for 2 layers and 4 layers. This is interesting and tells us that for small layer the ideal structure is bccSc - bccCr. It is too soon to tell what the ideal structure is for eight layers because I was unable to calculate the structure that I started from fccSc - bccCr with eight layers. However, for big number of layers Sc seems more likely to go to bct structure and for less number of layers Sc is more likely to go to fct structure. For all systems Cr keeps bcc structure with small deviation at the interface with Sc.

4.3.2 18.4 degree shift

In figure 4.6 and 4.7 I show the original atom positions and the final positions after I relaxed the system.

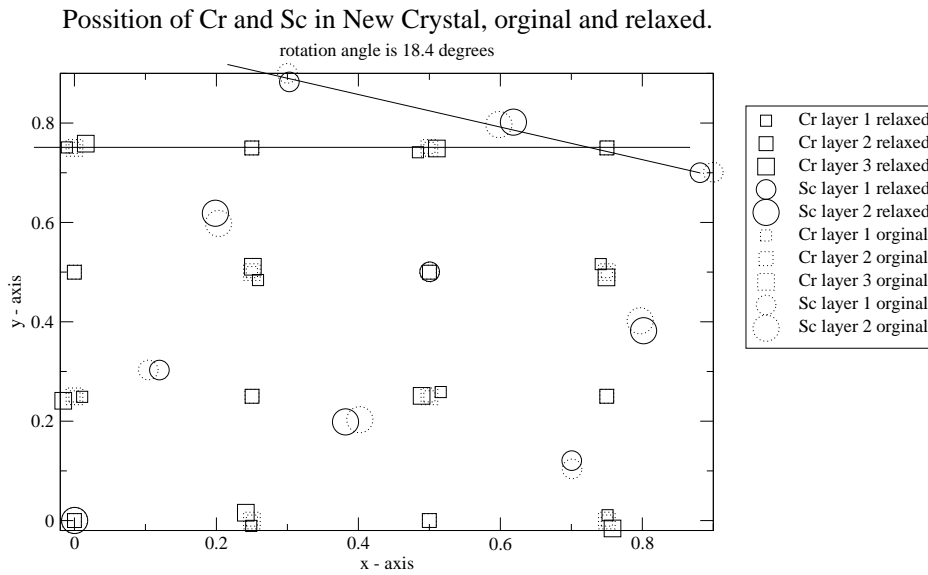


Figure 4.6. The position change for 18.4° model for xy - direction

Figure 4.6 shows the new crystal with 18.4° shift from the x-y view. The original positions of the atoms are the dotted squares and the dotted circles and the positions of the relaxed system are the squares and circles drawn with a full line. The smaller circles and squares lie deeper in the crystal than the bigger ones, which is illustrated in figure 4.7.

Figure 4.7 shows the new crystal with 18.4° shift from the z-y view. The

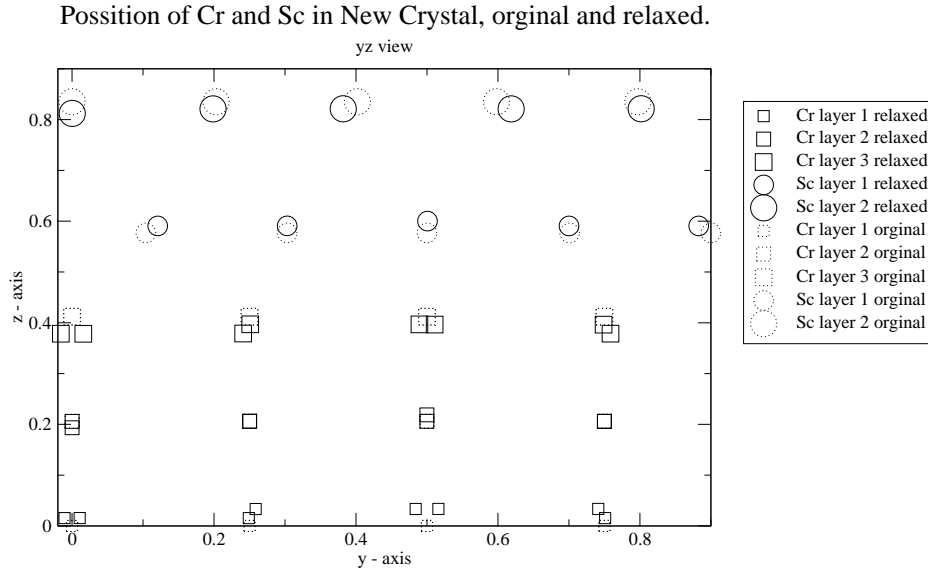


Figure 4.7. The position change for 18.4° model for yz - direction

original positions of the atoms are just like in figure 4.6, the dotted squares and circles. The positions of the relaxed system is the squares and circles drawn with a full line. There is no difference in showing the crystal from z-x view instead of z-y view. I choose to show it from the z-y side.

As you can see in figure 4.6 and 4.7 my pre calculations of the atoms' positions were good because they are close to the final positions. This make the calculations easier to converge. When I know that my starting positions are close to the final positions I can have hopes that a total energy calculation for a system with more layers will converge.

4.3.3 Interface energy per interface area

I have calculated the interface energy of Sc-Cr multilayers by calculating the difference between total energy and bulk energy. I could not calculate the interface energy for 8fccSc-8bccCr because VASP did not converge, perhaps there were too many atoms in the primitive cell. Computer power also stopped me from calculate structures of bcc-Sc on bcc-Cr for 18.4 degree shift with more than 2 layers.

Figure 4.8 shows the interface energy per interface area versus the number of layers. In the figure we see three lines. The one with circles is based on bcc-Sc - bcc-Cr with a 45 degree shift, the one with squares are based on fcc-Sc - bcc-Cr with 45 degree shift and the one with triangles are based on the new crystal with 18.4 degree shift.

As you can see in figure 4.8 I found that for only one layer of Sc and one and a

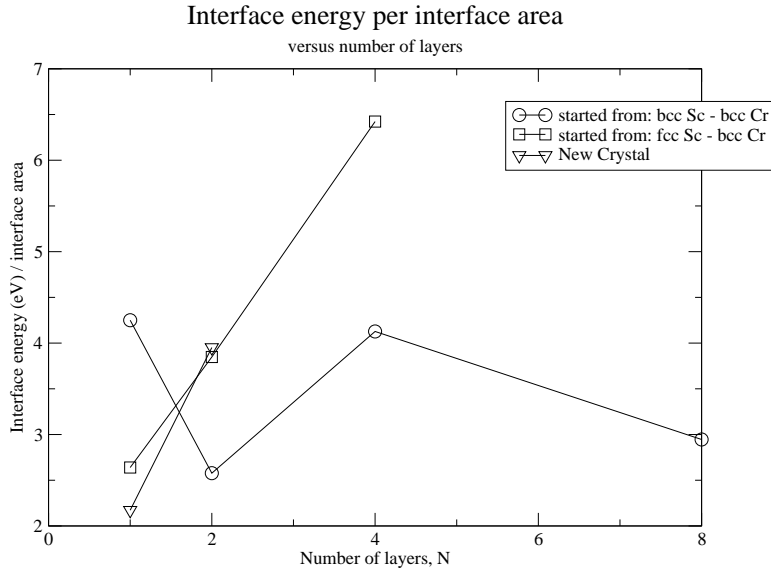


Figure 4.8. Interface energy per interface area

half layer of Cr the structure with 18.4 degree shift is the one that costs the lowest amount of energy to put together. But for two layers and more it is better to use a 45 degree shift with bcc-Sc and bcc-Cr. This indicates that a more amorph structure is better for small number of layers.

Cr is a much more stiff material than Sc which we can see in figure 4.5 when bcc based Sc goes from bcc to bct structure with an increasing number of layers. As discussed in section 4.2.2, Sc has an optimal lattice constant of 3.65 Å, in bcc structure ($a_{Sc} = 3.65 \text{ \AA}$). But in a system with Cr as in figure 4.2 and 4.3, Cr is forcing Sc to a lattice constant of $\sqrt{2} * a_{Cr} = 4.12 \text{ \AA}$. So putting bcc-Cr and bcc-Sc together is enlarging the Sc structure. When we increase the number of layers we have Sc atoms at a longer distance from Cr atoms which makes the Sc atoms more free, so they decrease their inter atomic distances. This is what we see in figure 4.5 when the distance between the Sc atoms is decreasing when the number of layers is increasing.

The fact that we get $\frac{a_{Sc}}{a_{Cr}} = 1.15$ results in $a_{Sc} = 3.35 \text{ \AA}$ (we know from before that $a_{Cr} = 2.91 \text{ \AA}$). From internet site www.webelements.com we see that $a_{Sc}(hcp) = 3.309 \text{ \AA}$, which is really close to the a_{Sc} from figure 4.5. This may be an indication that Sc tends to form hcp structure.

Chapter 5

Summary

This is a short summary of my conclusions.

1. For the simplest interface models the interface energy increases with decreasing number of layers, from 8 to 4 number of layers. This is indicating an increasing force for amorphization at small multilayer thicknesses.
2. The interface energy is found to be smallest for the 18.4 degrees interface. This indicates a tendency in the system to form complex interfaces at small thicknesses.
3. Fcc based multilayers are clearly unstable at large thicknesses.
4. For bcc based multilayers with many layers, the structure is close to bct with c/a ratio of 1.15 inside the layer.

Chapter 6

Further work

6.1 Further work

First of all we have to model proper amorph multilayers which will be able to describe experimental data.

It would be nice to see what value there is on the interface energy of the structure with a 18.4 degree shift for 4 and 8 layers. And where the atoms between the interface layers go when we relax the system. Do they remain in bcc structure or do they move?

Another thing left to do is to generate a model that describes impurities of N, O etc. in the multilayer. We have to show how sensitive the mirror is to impurity.

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