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D1.3 Simulation of interface structures

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1 Introduction

The purpose of this deliverable is to simulate the structure of the interfaces between dissimilar materials, especially the interface of rare earth, spacer layer and transition metal substrates, e.g., for Gd/X/Fe heterostructures, where X can be 3d, 4d or 5d elements. The idea is to achieve realistic chemical compositions due to interdiffusion of atoms across the interfaces at elevated temperatures. So far, the Uppsala node has considered ideal interfaces (without interdiffusion) to predict suitable materials combinations to realize heterostructures with high saturation moments. To simulate realistic interfaces, a *Kinetic Monte Carlo* (KMC) code has been developed by the UPP node.

When an interface is grown experimentally, usually it is not atomically sharp. The atoms diffuse from one layer to other and hence, alloyed layers are formed. In this project, we have modeled a 3 layer interface structure using KMC simulations to study this diffusion at the interface with vacancy defects mediating the atomic diffusion.

2 Technical details and Algorithm

We have performed KMC simulations [Ref. 1] in a three-layered geometry, e.g., Fe/Cr/Gd containing vacancies that mediate the diffusion of atoms across the interfaces. At present, energy barriers ΔE are taken as model values, which will be eventually determined from *ab-initio density functional* calculations and will be included in the code. We have tested the code using a 100x100 lattice.

The technical details are the following:

i. size (x) = 100

ii. size(y) = 100

iii. size(z) = 3

iv. vacancy = 10%

v. Temperature = 100K, 400K, 800K, 1000K

vi. Number of steps = 10*size(x)*size(y)*size(z)

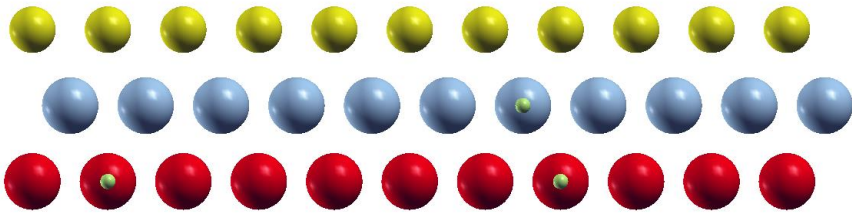


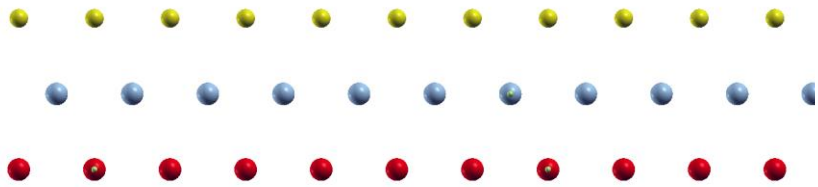
Illustration 1: Scaled down preview of the lattice in xz plane. The small green points are empty spaces. The system is scaled down for a better visualization.

The KMC algorithm is as follows.

1. Initialize the lattice
2. Form a list of all possible rates of the system (r_i) (4 here)
3. Calculate the cumulative rate $R_i = \sum_{j=1}^{i=N} r_i$. Let $R_N = R$, where N is the total number of particles in the system.
4. Generate a random number ρ_1= (0,1].
5. Find an event i such that $R_{i-1} < \rho_i < R_i$
6. Carry out the event i
7. Return to step 4.

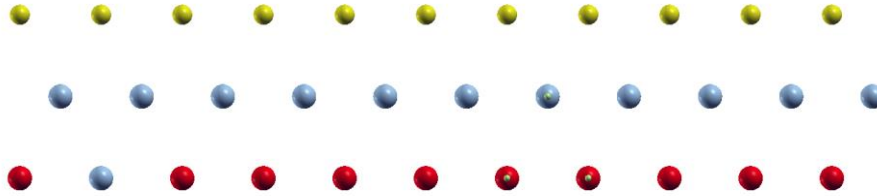
3 Results

Below, we show the simulated interface structures for different temperatures. As expected, diffusion increases with an increase in temperature. For these calculations, we have chosen the activation barriers as $\delta E_{layer1 \rightarrow layer2} = 0.4$, $\delta E_{layer2 \rightarrow layer3} = 0.6$. Below, we show the simulated structures at different temperatures, 100K, 400K, 800K and 1000K. One can clearly see the formation of highly interdiffused layers at high temperatures.



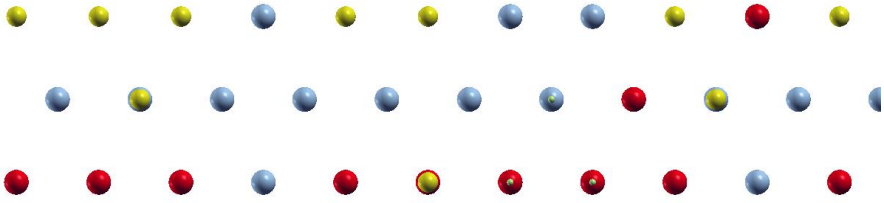
100 K

Illustration 2: T=100K



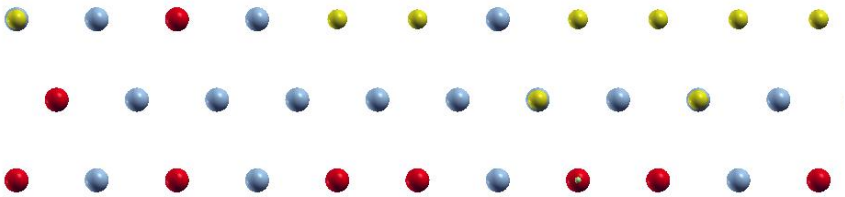
400 K

Illustration 3: T=400K



800 K

Illustration 4: T=800K



1000K

Illustration 5: T =1000K

4 Conclusion

To conclude, we have developed a Kinetic Monte Carlo code, which is capable of taking input from ab-initio calculations to calculate atomic diffusion across different interfaces of heterostructures comprised of rare earth and transition metal layers.

Currently, we are performing density functional calculations [Ref. 2] using the VASP code to calculate the diffusion barriers for Fe/Cr/Gd heterostructures. This is challenging as the atomic diffusion occurs through spin-dependent potential surfaces. As Cr and Gd are antiferromagnetically coupled similar to Fe and Cr, highly non-trivial scenarios occur involving spin flips along the diffusion path. We are in the process of stabilizing these calculations.

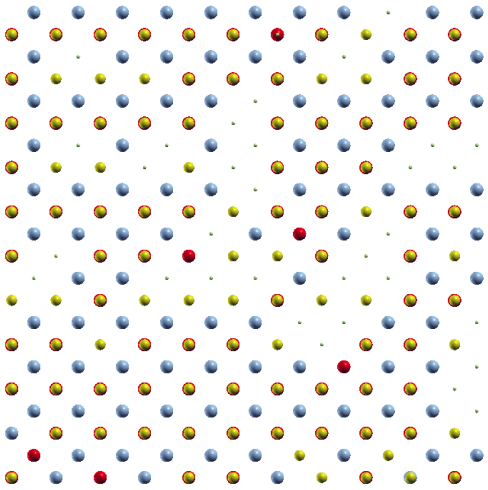


Illustration: Top view, T=1000K.
Empty sites denote vacancies.

5 References

1. A. F. Voter, Volume 235 of the series NATO Science Series pp 1-23, Radiation Effects in Solids, 2007
2. G. Kresse and J. Hafner, Phys. Rev. B **47** , 558 (1993); ibid. **49** , 14 251 (1994); G. Kresse and J. Furthmuller, Comput. Mat. Sci. **6** , 15 (1996).