Supplementary Information for "How interface properties control the equilibrium shape of core-shell Fe-Au and Fe-Ag nanoparticles"

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1 Au(111)/Fe(110) and Ag(111)/Fe(110) interfaces

DFT calculations were carried out on models of the X(111)/Fe(110) (x=Au or Ag) interfaces built using different coincidence networks to approximate the Nishiyama-Wasserman epitaxial relationship.[1] In this relationship, the mismatch between the Au(Ag) and Fe unit cells along the $[10\bar{1}]$Fe//$[1\bar{1}\bar{2}]$X direction is very large which is the reason why we approximate it by a coincidence network. In Tab. 1, we report the mismatch between the unit cells of Au(Ag) on Fe along the $[10\bar{1}]$Fe//$[1\bar{1}\bar{2}]$X and the one obtained with the coincidence networks that were used in the calculations. Due to the lattice mismatch between the X metal fcc lattice and the Fe bcc lattice obtained with DFT-PBE (see Tab. 1), two possible coincidence networks can be built along the $[10\bar{1}]$Fe//$[1\bar{1}\bar{2}]$X direction: one made of 7 X unit cells and 9 Fe unit cells (7x9) and one made of 8 X unit cells and 10 Fe unit cells (8x10). These two different networks have been relaxed for the Au(111)/Fe(110) interface only.

	Exp	DFT-PBE	EAM-LJ
Au/Fe unit cells	22.8%	27.5%	23.4%
8x10 Au/Fe	-	2.0%	-
7x9 Au/Fe	-	0.8%	-
18x22 Au/Fe	-	-	0.9%
Ag/Fe unit cells	23.4%	27.2%	24.1%
8x10 Ag/Fe	-	1.8%	-
18x22 Ag/Fe	-	-	1.5%

Table 1 Values of the mismatch (in %) between X (X= Au, Ag) and Fe along the $[10\bar{1}]$Fe//$[1\bar{1}\bar{2}]$Ax direction in the X(111)/Fe(110) interface.

After relaxation, the interface exhibits a network of interface dislocations shown in Fig.1. For both coincidence networks, we observe two interface dislocations separated by 4 Fe atomic columns on one side and by 5 Fe atomic columns (for the 7x9 network) or 6 Fe atomic columns (for the 8x10 network) on the other side. Between the two dislocations separated by 4 atomic columns, the Fe atoms at the interface present important displacements along the direction perpendicular to the interface (z-axis) which amplitude is of 0.37 Å for the 7x9 network and of 0.40 Å for the 8x10 one. In the largest interval between consecutive dislocations, these displacements are absent. Energetically, the interface model with the 8x10 coincidence network is found lower by 67 meV than that with the 9x11 one. Therefore, the former one has been selected and it was used for the Ag(111)/Fe(110) interface model. In the latter case, we found a similar dislocation network with atomic z-displacements of 0.31 Å .

For the X(111)/Fe(110) interface computed with the EAM-LJ potential, the coincidence network is slightly different than for the DFT case because the lattice mismatch is not the same (Tab. 1). For this reason, we used a lattice network of 9 X unit cells for 11 Fe unit cells. Moreover, in the interface model used to compute the interface energy, this network was doubled in the $[10\bar{1}]$Fe//$[1\bar{1}\bar{2}]$X direction. After relaxation, the interface exhibits a network of dislocations separated by 4 Fe columns on one side and 7 Fe columns on the other side, for both systems (Au/Fe and Ag/Fe). As for the DFT case, we observe significant displacements of the Fe atoms perpendicular to the interface between the dislocation separated by 4 Fe columns, of 0.44 Å for Au/Fe and of 0.32 Å for Ag/Fe. These values are in very good agreement with the values obtained by DFT.

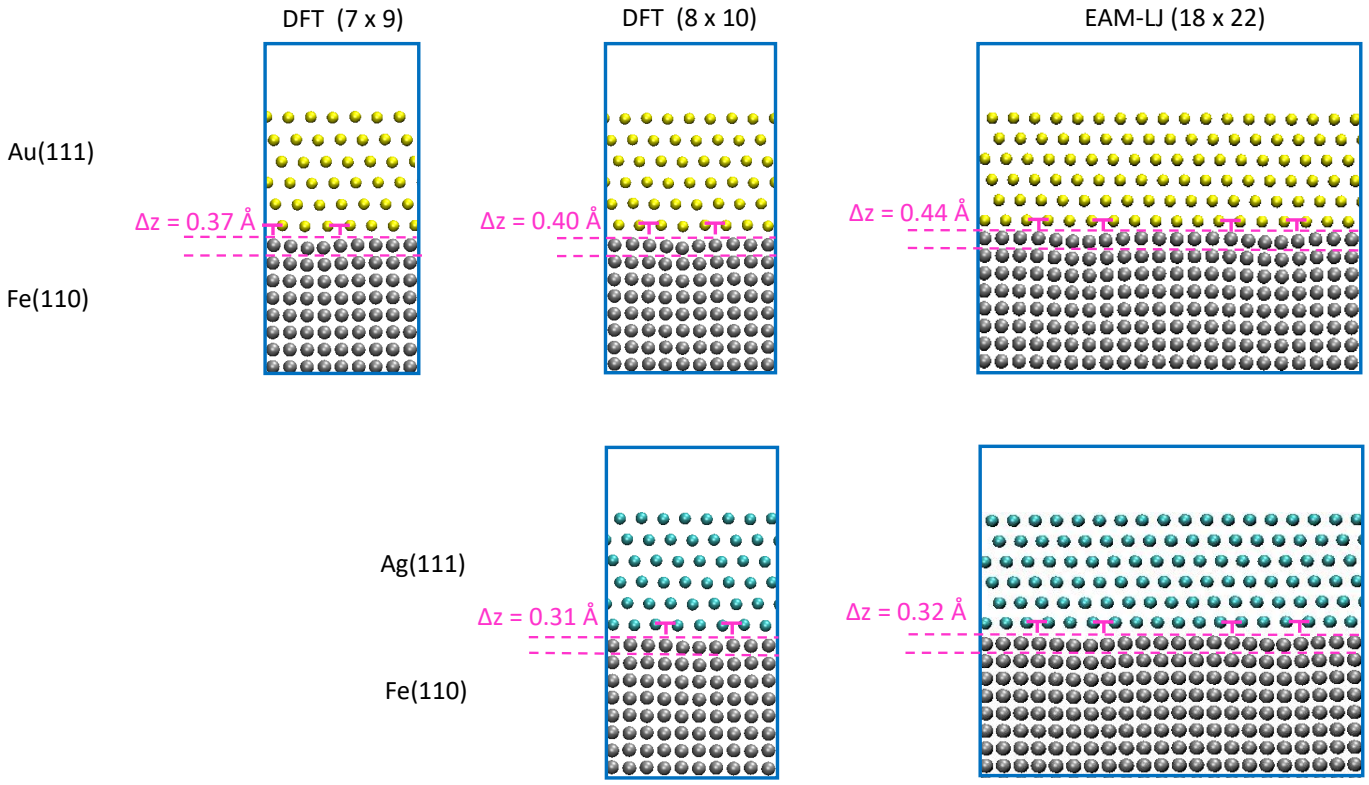

Fig. 1 Atomic positions after relaxation for the Au(1110/Fe(110) (top line) and Ag(111)/Fe(110) (bottom line) interface models used to compute the interface energies. The different tested coincidence networks are shown for the DFT-PBE and EAM-LJ calculations. Δz indicates the largest atomic displacements of the Fe atoms along the direction perpendicular to the interface.

Notes and references

1 E. Bauer and J. H. van der Merwe, *Physical Review B*, 1986, **33**, 3657–3671.

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