Determination of lattice distortion in nanoparticles on strained substrates using molecular dynamics

J. Zhou, S. Saranu and U. Herr
Institute of Micro- and Nanomaterials, Ulm University, 89081 Ulm, Germany
E-mail: saranu.rao@uni-ulm.de

Abstract. Magnetoelastic anisotropies arising from substrate induced strains provide a way to optimize the magnetic properties of nanoparticles. A possible way to induce such anisotropies is the deposition of clusters on substrates which are deformed or otherwise expanded subsequently. However, the experimental determination of strain in nanoparticles is complicated by the low diffraction intensities. We used the molecular dynamics simulation technique to determine the deformation of Co particles deposited on Cu substrates. Co particles of 4.5 nm diameter with fcc structure were built using a Wulff construction and subsequently deposited with their (111) or (100) facets on (100) oriented Cu substrates with a kinetic energy of 10 meV/atom at temperatures of 10 K or 300 K. After the deposition, the lattice parameter of the Cu substrate has been increased continuously. It is found that significant strain in the Co particles can only be obtained in the case of (100) facets on (100) surfaces at low temperatures.

1. Introduction
Ferromagnetic nanoparticles are promising candidates for ultrahigh-density magnetic data storage in patterned media [1]. The storage density is presently limited by the onset of superparamagnetism at very small particle size. A possible solution is the use of materials with extremely high crystalline anisotropy such as ordered FePt. However, the ordering of these particles requires annealing at elevated temperatures which may lead to agglomeration and growth. An alternative approach would be to increase the total magnetic anisotropy by adding further anisotropies such as shape anisotropy or magnetoelastic anisotropy. It has recently been demonstrated that magnetoelastic anisotropies can lead to a 100% enhancement of the perpendicular magnetic anisotropy in CoPd multilayer systems suitable for perpendicular recording [2]. In those experiments, the CoPd multilayers were deposited on Ta foils which could be loaded with hydrogen after the deposition. First experimental results have shown that it is difficult to determine the actual strain or stress in the nanoparticles by X-ray diffraction due to the low scattering intensities. Therefore, we have done a molecular dynamics study of Co nanoparticles on different substrates in order to investigate the theoretically possible strain transfer from substrate to nanoparticles during the expansion of the substrates (which would be achieved by hydrogen loading in the experiments).

2. Methods
The Co nanoparticles consisted of 4712 atoms, and the size of the Cu substrate was 54000 atoms with a free (100) surface. We used the TB-SMA potential proposed by Cleri and Rosato [3] to describe the Cu-Cu, Co-Co and Cu-Co atomic interactions. Coefficients for these three interactions were taken
from Mazzone and Rosato[4]. As in previous work on cluster deposition processes[5, 6], two layers of substrate boundary atoms were fixed (except for the free surface), and two additional layers next to the boundaries served as a heat bath to maintain a specified ambient temperature (10K or 300K) by velocity scaling. The time step was 3fs and the equations of motion were integrated using a fourth-order Gear algorithm. Previous research shows that small Co particles in equilibrium prefer fcc structures rather than hcp expected for bulk Co [7]. The fcc Co particle in our simulation was built with a Wulff shape (about 4.5 nm diameter with eight (111) facets and six (100) facets) determined by minimizing the surface energy of the Wulff polyhedron.

In a first step, the fcc Co particle, while located above the Cu (100) surface far enough to prevent interaction, experiences a short-time relaxation at the specified temperature. Afterwards an additional velocity corresponding to a kinetic energy of 10meV/atom pointing to the substrate surface was applied, leading to collision of the particle with the substrate surface. The cluster orientation was chosen such that either the (100) or the (111) facet was parallel the substrate surface during the impact. It was found that after 90ps a quasi-equilibrium situation was reached (it must be noted here that on longer time scales a burrowing of the clusters by diffusion processes will take place). In the second step, the Cu substrate was isotropically expanded up to 8% linear strain by continuously increasing its equilibrium lattice parameter over 150ps, equivalent to a strain rate of 5.33x10^8 s^1.

The structure of the nanoparticles was analysed by calculating the structure factor from the atomic positions. The as-deposited Co particles were always tilted to some degree with respect to the initial orientation before the impact. In order to determine the precise orientation of the particle we used a scheme similar to X-ray rocking curve measurements. The tilt of the cobalt particle with respect to the substrate surface was determined by evaluation of the intensity scattered into a certain direction, where the scattering vector q has a constant magnitude corresponding to the approximate value of the interplanar spacing of interest, but a variable direction. The particle orientation is then determined from the direction where the intensity maximum occurs. The precise value of interplanar spacing is obtained by searching the maximum intensity for fixed direction and variable magnitude of q. In addition, to study the internal structure of the final configuration, the bond-order method [8] was used to identify three local crystalline structures: fcc, hcp and non 12-fold coordinated atoms. The atomistic visualization software AtomEye[9] was employed to display different views.

3. Results

We have simulated impact of the Co particles on either (100) or (111) facet at temperatures of 10K or 300K. Due to the small misfit between the Cu and the Co lattice parameters, impact on the (100) facet results in a coherent interface, whereas for the impact on (111) facet an incoherent interface is expected. The interface structure can be observed in configuration snapshots taken after landing of the Co particles shown in fig. 1. As expected for the two cases with coherent interface, the Co atoms at the interface align perfectly with the Cu lattice (Fig. 1 (c) and (e)). However, this alignment was even observed for the other two cases with incoherent interface (Fig. 1 (d) and (f)). The adjacent layers of Co atoms remain in the (111) plane configuration, and the transition between both types of Co planes is accompanied by a tilt of the whole particle as seen in Fig. 1 (b). The overall structure of the landed Co particles as determined from the simulated diffraction patterns is perfect fcc. Only in the case of impact on the (100) facet at 300K, several layers with local hcp structure were found (Fig. 2). These layers correspond to three (111) slip planes with different orientation as indicated in Fig. 2(c). The formation of these stacking-fault like defects is probably facilitated by the low value of the stacking-fault energy of Co (about 18.7mJ/m² based on the scheme proposed by Meyer and Lewis [10]).

During subsequent strain application by isotropic expansion of the Cu substrate, we found that strain could only be transferred effectively to the part of the landed particle adjacent to the interface (lower part). For a more detailed evaluation the particle was divided into three parts containing equal number of atoms along the out-of-plane direction. The strain perpendicular to the interface was characterized for each part separately by monitoring the interplanar distance of the (200) (for impact on (100) facet) or (111) Co planes (for impact on (111) facet).
**Figure 1.** Snapshots of the Co particle deposition. The darker spheres represent Co atoms and the lighter ones denote Cu atoms. (a) Impact on (100) facet at 10K, (b) impact on (111) facet at 10K, both viewed from <110>. The dashed box in (a) marks the interface region containing one Co layer and one Cu layer; (c) top view of this region for (100) impact at 10 K. Interface structures in (e), (d) and (f) correspond to (100) impact at 300K, (111) impact at 10K and (111) impact at 300K, respectively.

**Figure 2.** Structure of Co particle after impact on (100) facet at 300 K. Atoms with local hcp structure are visualized by specifying a larger radius and lighter colour. (a) Viewed from <110>; (b) rotated to see all three planes; (c) extracted from (b) to see the relative position and size of the three (111) planes. Note that every plane terminates when it intersects with another one.

Fig. 3 shows the variation of the interplanar distance for the impact on the (100) facet at 10 K. Whereas the lower part of the landed Co particle deformed significantly, the deformations in other parts as well as the average change in the whole particle are very small. The two different values at zero strain for the lower part correspond to the state before and after particle deposition, respectively. Oscillations of the interplanar distance with increasing substrate strain are observed, most prominently in the middle part. These oscillations are associated with energy releases at the same strain values, indicating the formation of defects. However, no extended defects such as stacking faults have been observed during deformation at 10 K.

Fig. 4 shows a comparison of the calculated strain in the parts adjacent to the substrate interface for the different impact conditions. Significant strain transfer is observed only for the case of impact on
the (100) facet at 10K. The fact that strain in this case increases roughly proportional to the substrate deformation indicates purely elastic deformation up to 8% linear strain of the substrate. This may be attributed to the coherent nature of the Co-Cu interface. On the other hand, the absence of elastic deformation for the same configuration at 300 K indicates the importance of thermally activated processes for the deformation of the nanoparticles. This conclusion is further supported by the occurrence of the stacking faults (possibly as a result of partial dislocation motion) after deposition at 300K, but not after deposition at 10 K. In the case of the incoherent Co-Cu interfaces, plastic deformation may be facilitated by the defect structure of the interface associated with the tilt of the particles. The exact nature of these defects is subject of further investigations.

![Figure 3](image1.png)

**Figure 3.** Interplanar distances of (200) Co planes in different parts of the Co particle after (100) impact and substrate expansion.

![Figure 4](image2.png)

**Figure 4.** Strain transfer to the parts adjacent to the substrate interfaces of the deposited Co particles for the different impact conditions.

4. Conclusion
We have studied the possibility of inducing deformations in substrate supported nanoparticles by transferring strain from the substrate to the particles. For Co particles on Cu (100) surfaces significant deformation of the particles occurs only at low temperatures and for a coherent interface. In the presence of defects, no significant elastic deformation has been found. Although only a few selected configurations have been studied here it may be concluded that strain transfer is difficult in general in the case of free particles deposited on surfaces. Further studies of partially of fully buried particles [11, 12], or particles covered with additional layers after deposition are necessary to evaluate the potential of the strain-transfer approach.

Acknowledgments
This research was supported by the Landesstiftung Baden-Württemberg.

5. References
[1] Sun S, Murray C B, Weller D, Folks L and Moser A 2000 Science 287 1989
[2] Mohanan S and Herr U 2007 J. Appl. Phys 102 093903
[3] Cleri F and Rosato V 1993 Phys. Rev. B 48 22
[4] Mazzone G, Rosato V and Pintore M 1997 Phys. Rev. B 55 837
[5] Frantz J and Nordlund K 2003 Phys. Rev. B 67 075415
[6] Haberland H, Insepov Z and Moseler M 1995 Phys. Rev. B 51 11061
[7] Kitakami O, Sato H, Shimada Y, Sato F and Tanaka M 1997 Phys. Rev. B 56 13849
[8] Chushak Y and Bartell L S 2001 Eur. Phys. J. D 16 43
[9] Meyer R and Lewis L J 2002 Phys. Rev. B 66 052106
[10] Zimmermann C G et al. 2001 Phys. Rev. B 64 085419
[11] Zimmermann C G et al. 1999 Phys. Rev. Lett. 83 1163

The 13th International Conference on Rapidly Quenched and Metastable Materials IOP Publishing
Journal of Physics: Conference Series 144 (2009) 012010 doi:10.1088/1742-6596/144/1/012010