The stability of phases at finite temperatures is given by the free energy. But the fact that it is not expressible in terms of ensemble averages over functions of position and velocity coordinates, complicates its determination in atomistic simulations. In order to overcome this problem, thermodynamic integration methods are used. This method is not limited to thermodynamic paths which can be followed in experiments. Often artificial paths along which the inter-particle interaction is switched off, lead to much better results.

Here we calculate the free energy of iron nano clusters along a thermodynamic path starting from the embedded atom model and ending up in a set of three dimensional harmonic oscillators. The results allow to arrange the various morphologies in a phase diagram of temperature and number of atoms. The phase boundaries, which are normally hidden in between hysteresis loops, can be determined very accurately from the intersection of the free energies of the competing morphologies. As examples, we analyse three common morphologies, namely the icosahedron, the cuboctahedron with fcc structure and its Bain transformation to the bcc structure. Additionally the new shellwise Mackay transformed morphology reported in Phys. Rev. Lett. 99 083402 is taken into account.