Appendix C: Some Numerical Issues

This appendix concerns numerical issues associated to the functional form for the s-embedding terms. As shown in Equation (20), we chose a typical second moment expression, characterized by a square root dependence of the density. Derived in its original framework [37], for the bulk of a material, this expression is never evaluated near zero density. However, given the specific conditions of the s-density functions for the application to the alloy (see Equation (17)), the s-density can reach values close to zero in a dilute alloys, meaning that the forces due to the s-embedding function become singular.

Frequently, potentials are tabulated on a grid of ~5000 points between the extreme values of the density (as a conservative estimate, we take 0 and 1, which are the extremes for our s-density on a perfect lattice). Such tables, in turn, are typically interpolated by cubic splines to obtain values in between grid points. A comparison of such an interpolation with the analytic expression is given in Figure C.1 for the Fe s-embedding function. Clearly, due to the cusp of the square root, there is a deviation of ~0.6 meV between the interpolated and analytic expression in the first interval, while starting from the second interval, the difference is negligible. If we now take bulk Fe with an isolated Cr atom, the Fe atoms in the 4nn and 5nn shells from the Cr atom take a value for the s-density in the first interval of the tabulation, as indicated by the arrows in Figure C.1. When computing the total energy of the latter system, we find a discrepancy of ~20 meV due to the spline interpolation of the s-embedding function.

We can thus conclude that a typical tabulation of the s-embedding function introduces a non-negligible systematic error of ~20 meV in the total energy per isolated Cr atom added to the Fe matrix. Therefore, special care must be taken to compute the energy and force contribution of the s-embedding terms and we recommend that the proper analytic expression is used to describe the s-embedding functions, rather than tabulations.

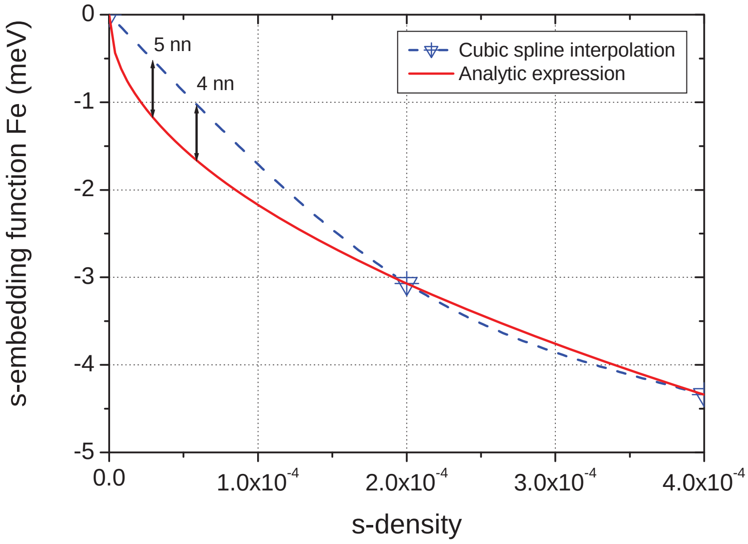

Figure C.1 – Comparison between the analytic expression for the Fe s-embedding function with a cubic spline expansion on a typical grid.