Influence of long-range C-C elastic interactions on the structural stability of dilute Fe-C solid solutions

The thermodynamical and structural description of solid solutions is challenging due to the long-range character of the interatomic interactions, originating from the slow decay of the displacement field. Here we employ the reciprocal space Krivoglaz-Kanzaki force concept\(^1\) to calculate the long-range elastic interaction between C interstitials in dilute Fe-C solid solutions. In this analytical approach the Kanzaki forces and the lattice Greens function are expressed by lattice parameters, elastic constants and coefficients, describing the concentration dependence of the impurity induced distortions of the Fe matrix. The parameters entering the analytical approach are obtained atomistically using an EAM potential.\(^2\) Our study predicts the stability of an orientationally ordered, tetragonally deformed phase of the Fe-C solid solution. The critical concentration for the tetragonal-cubic transition at room temperature is found in excellent agreement with recent experimental data. The developed multi-physics methodology is straightforward to combine with ab initio methods and can be readily applied to other solid solutions.


For more information contact Dr. Rebecca Janisch, rebecca.janisch@rub.de