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Pair Interaction in Transition-Metal Nanoparticles

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Abstract : Pair-interaction approximations allow to consider a different states of condensed matter from a single position. At the same time, description of an effective pair interaction in transition metal is a hard task since the d-electron contribution to the potential energy in this case is non-pairwise in principle. There are a number of models for transition-metal effective pair potentials. Here we use the Wills-Harrison (WH) approach to calculate pair potentials for Fe, Co, and Ni in crystalline, liquid, and nano states. Last is especially interesting since nano particles of pure transition metals immobilized on the dielectric matrices are widely used in different fields of advanced technologies: as carriers and transmitters of information, as an effective catalytic materials, etc. It is found that the minimum of the pair potential is deeper and oscillations are stronger in nano crystalline state in comparison with the liquid and crystalline states for all metals under consideration.

Keywords : effective pair potential, nanocrystalline state, transition metal, Wills-Harrison approach
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