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Precise EXAFS approaches to invar alloys and negative thermal expansions

Thermal expansion of FeNi Invar and zinc-blende CdTe was investigated from the view point of local structure using the EXAFS spectroscopic data and the path-integral effective classical potential (PIECP) Monte Carlo computational simulations. First, the quantum statistical perturbation theory is intuitively described to see different character concerning thermal expansion between the quantum and classical theories. Second, the PIECP theory is briefly described to note advantages and disadvantages of this simulation technique. Subsequently, the results of the FeNi Invar alloy are summarized. The origin of zero thermal expansion in the FeNi alloy is ascribed to the so-called Invar effect that implies the variation of the electronic structure of Fe atoms depending on temperature. Zero thermal expansion at low temperature is however found to originate from the vibrational quantum effect. It is also noted that the interatomic distances of Fe-Fe, Fe-Ni, and Ni-Ni pairs are slightly but meaningfully different from each other, although the alloy exhibit a simple fcc crystal. Such a pair-dependent difference is also true for thermal expansion and we will discuss thermal expansion from the local point of view, which is interestingly different from the lattice thermal expansion significantly. Finally, the results of the zinc blende (or diamond) structure are presented. Although the origin of negative thermal expansion in these tetrahedral crystals is known as a result of classical vibrational anomaly within the Newton dynamics theory, the quantum statistical simulation is found to be essential to reproduce the negative thermal expansion of CdTe. It is emphasized that the vibrational quantum effect and classical anharmonicity are of great importance for the understanding of low-temperature thermal expansion as well as the elastic constants.

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