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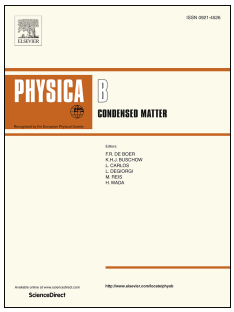

Dependence of cumulants and thermodynamic parameters on temperature and doping ratio in extended X-ray absorption fine structure spectra of cubic crystals

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Dependence of cumulants and thermodynamic parameters on temperature and doping ratio in extended X-ray absorption fine structure spectra of cubic crystals

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Abstract: The thermodynamic properties and anharmonic perturbation factor of orderly doped crystals are described in terms of the cumulants in extended X-ray absorption fine structure (EXAFS) spectra. The thermodynamic parameters and cumulants are studied based on the anharmonic correlated Einstein model. We derive analytical expressions for the dispersion relation, the correlated frequency and Einstein temperature, and the EXAFS cumulants. Parameters of the Morse potential, thermal expansion coefficient due to effect of anharmonicity, anharmonic factor, the EXAFS phase including the anharmonic effects depend on doping ratio of cubic-structure crystals are considered. The derived anharmonic effective potential includes the contributions of all the nearest neighbors of the absorbing and scattering atoms to account for three-dimensional interactions and the parameters of the Morse potential to describe single-pair atomic interactions. Numerical results for face-centered cubic (fcc) crystals of copper (Cu-Cu) and silver (Ag-Ag) and their compound Ag-Cu agree reasonably with experiments and other theories.

Keywords: anharmonic; EXAFS; cumulants; thermodynamic; doping ratio.

1. INTRODUCTION

To study how the cumulants, thermal parameters, and thermodynamic properties of lattice crystals of a substance depend on the temperature and their doping ratio (DR), in previous studies we have used extended X-ray absorption fine structure (EXAFS) spectra, an approach that has developed into a powerful probe of the atomic structures and thermal effects of substances.[1,3,4,6–11] The functions of EXAFS spectra provide information about the atomic number of each shell, and their Fourier magnitudes provide information about the radius of this atomic shell.[1,4,8,9] The thermodynamic parameters and the EXAFS cumulants up to third order have been derived for pure cubic crystals by using the anharmonic correlated Einstein model (ACEM) in EXAFS theory.[7,9] However, the thermodynamic parameters, cumulants, anharmonic perturbation factor, and thermal expansion coefficient for doped face-centered cubic (fcc) crystals, such as crystals of copper (Cu) doped with silver (Ag) (Ag-Cu), are yet to be determined.

In the present study, we use the anharmonic effective Einstein potential in EXAFS theory[7] to formulate thermodynamic parameters such as the effective force constant, anharmonic factor, thermal expansion coefficient, cumulant expressions, and some other parameters such as the

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