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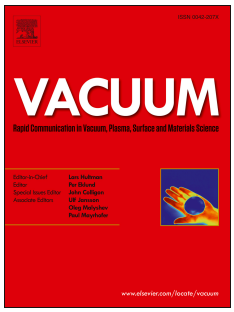

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ANHARMONIC EFFECTS OF GOLD IN EXTENDED X-RAY ABSORPTION FINE STRUCTURE

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Abstract:

The anharmonic effects of gold in extended X-ray absorption fine structure (EXAFS) have been investigated through the consideration of the first four EXAFS cumulants up to temperature 800 K within the anharmonic correlated Debye model. The interatomic potential between two intermediate atoms has been described by the second-moment approximation to the tight-binding model and its parameters were determined from first-principles calculations. Our results of the first four EXAFS cumulants and anharmonic effective potential are compared with those of experiments showing the good and reasonable agreements. We have shown in detail that the anharmonicity contributions of the thermal vibration of atoms are important to EXAFS cumulants at high temperature.

Keywords: Anharmonicity, gold, EXAFS, Cumulant, Debye-Waller factor

INTRODUCTION

The extended X-ray absorption fine structure (EXAFS) spectroscopy is a powerful technique for investigating local structures of crystalline as well as amorphous materials [1,2]. It provides apparently different structural information such as bond distances, coordination number and geometry at various high temperature due to anharmonicity [3,4]. This technique can be used independently or in coordination with X-ray crystallography or nuclear magnetic resonance spectroscopy [1]. The formalism for including anharmonic effects in EXAFS is often written on the basis of the cumulant expansion approach as [5,6]

$$\chi(k)=\frac{F(k)}{kR^2}e^{-2R/\lambda(k)}\,\mathrm{Im}\left\{e^{i\varphi(k)}\exp\left[2ikR+\sum_n\frac{(2ik)^n}{n!}C_n\right]\right\}, \quad (1)$$

where k and λ are, respectively, the wave number and mean free path of emitted photoelectrons, $F(k)$ is the real atomic backscattering amplitude, $\varphi(k)$ is net phase shift, the thermal average distance $R=\langle r\rangle$ with r is the instantaneous bond length between absorbing and backscattering atoms, and $C_n\,(n=1,2,3,...)$ are the EXAFS cumulants. The cumulant method allows the characterization of the first coordination shell in terms of parameters which describe the distance distributions as the first cumulant C_1 is the mean value which describes the net thermal expansion or disorder; the second cumulant C_2 is the variance which characterizes the Debye-Waller factor [7,8]; the third cumulant C_3 measures the distribution asymmetry which describes the asymmetry of the pair distribution function; and the fourth cumulant C_4 measures the flatness of distribution function and gives the anharmonic contribution to EXAFS amplitude [9,10].

There are many methods that have been developed in order to study the temperature dependence of EXAFS cumulants such as path-integral effective-potential theory [11], statistical moment method [12], Debye model [13] and Einstein model [14]. A simple