Pressure effects in DebyeWaller factors and in EXAFS

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Abstract: Anharmonic correlated Einstein model (ACEM) and statistical moment method (SMM) have been developed to derive analytical expressions for pressure dependence of the lattice bond length, effective spring constant, correlated Einstein frequency and temperature, DebyeWaller factors (DWF) or second cumulant, first and third cumulants in Extended X-ray Absorption Fine Structure (EXAFS) at a given temperature. Numerical results for pressure-dependent DWF of Kr and Cu agree well with experiment and other theoretical values. Simulated EXAFS of Cu and its Fourier transform magnitude using our calculated pressure-induced change in the 1st shell are found to be in a reasonable agreement with those using X-ray diffraction (XRD) experimental results.
Author Keywords: DebyeWaller factors and cumulants; EXAFS; Pressure dependence effects
Index Keywords: Analytical expressions; Anharmonic; Cumulants; Debye Waller factor; EXAFS; Extended X-ray absorption fine structures; Lattice bonds; Numerical results; Pressure dependence; Pressure dependence effects; Spring constants; Statistical moments; Theoretical values; Bond length; Fourier transforms; Krypton; X ray diffraction; Pressure effects

Year: 2011
Source title: Physica B: Condensed Matter
Volume: 406
Issue: 3
Page : 456-460
Link: Scorpus Link
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ISSN: 9214526
CODEN: PHYBE
DOI: 10.1016/j.physb.2010.11.012
Language of Original Document: English
Abbreviated Source Title: Physica B: Condensed Matter
Document Type: Article
Source: Scopus
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References:

- (1988), E.D. Crozier, J.J. Rehr, R. Ingalls, D.C. Koningsberger, R. Prins, Wiley New YorkBunker, G., (1983) Nucl. Instrum. Methods, 207, p. 437
- Hung, N.V., Duc, N.B., Frahm, R.R., (2003) J. Phys. Soc. Jpn., 72, p. 1254
- Ingalls, R., Garcia, G.A., Stern, E.A., (1978) Phys. Rev. Lett., 40, p. 334
- Ingalls, R., Crozier, E.D., Whitemore, J.E., Seary, A.J., Tranquada, J.M., (1980) J. Appl. Phys., 51, p. 3158
- Freund, J., Ingalls, R., Crozier, E.D., (1989) Phys. Rev. B, 39, p. 12537
- Di Cicco, A., Filipponi, A., Itie, J.P., Polian, A., (1996) Phys. Rev. B, 54, p. 9086
- Polian, A., Itie, J.P., Daartyge, E., Fontaine, A., Tourillon, G., (1989) Phys. Rev. B, 39, p. 3369
- Hung, V.V., Hieu, H.K., Masuda-Jindo, K., (2010) Comut. Mater. Sci., 49, pp. S2417
- Rehr, J.J., Mustre De Leon, J., Zabinsky, S.I., Albers, R.C., (1991) J. Am. Chem. Soc., 113, p. 5135
- (1972) American Institute of Physics Handbook, , 3rd ed. AIP New York
- Tang, N., Hung, V.V., (1988) Phys. Status Solidi B, 149, p. 511
- Masuda-Jindo, K., Hung, V.V., Tam, P.D., (2003) Phys. Rev. B, 67, p. 094301
- Erkoc, S., (1997) Phys. Rep., 278 (2), p. 81
- Hung, V.V., Hoa, N.T., Lee, J., (2006) AJSTD, 23 (1-2), p. 27
- Hung, V.V., Masuda-Jindo, K., (2000) J. Phys. Soc. Jpn., 69, p. 2067
- Hung, N.V., Rehr, J.J., (1997) Phys. Rev. B, 56, p. 43
- Ramakrishnan, J., Boehler, R., Higgins, G.H., Kennedy, G.C., (1978) J. Geophys. Res., 83, p. 3535
- Pirog, I.V., Nedoseikina, T.I., Zarubin, A.I., Shuvaev, A.T., (2002) J. Phys.: Condens. Matter, 14, p. 1825
- Vila, F.D., Rehr, J.J., Rossner, H.H., Krappe, H.J., (2007) Phys. Rev. B, 76, p. 014301
- Daniel, M., Pease, D.M., Van Hung, N., Budnick, J.I., (2004) Phys. Rev. B, 69, p. 134414
- Hung, N.V., Fornasini, P., (2007) J. Phys. Soc. Jpn., 76, p. 084601
- Hung, N.V., Tien, T.S., Hung, L.H., Frahm, R.R., (2008) Int. J. Mod. Phys. B, 22, p. 5155
- Walzer, U., Ullmann, W., Pan'Kov, V.L., (1979) Phys. Earth Planet. Inter., 18, p. 1
- Feynman, R.P., (1972) Statistical Mechanics, , Benjamin Reading, MA
- Girifalco, L.A., Weizer, V.G., (1959) Phys. Rev, 114, p. 687

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