

Microsymposium

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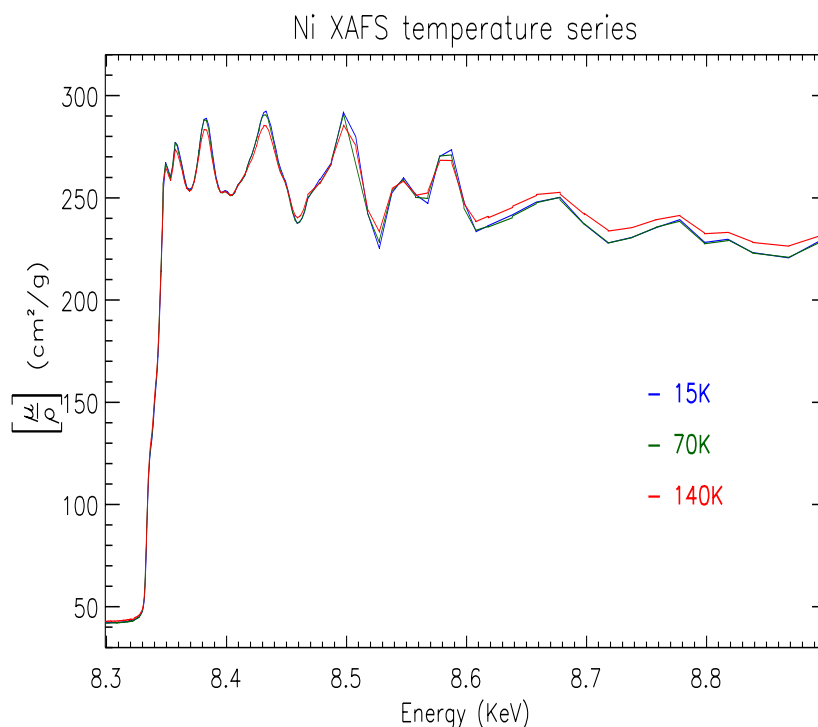
An XAFS Investigation of static and thermal disorder above the Nickel K-edge

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We present recent experimental X-ray Absorption Fine Structure (XAFS) data of the Nickel K-edge, measured at temperatures of 15, 70 and 140 K. This study has taken elements of the X-ray Extended Range Technique (XERT) and for the first time, applied them to a cryostat cold cell system. These measurements permit critical tests of XAFS theory, with emphasis on quantification of the Debye-Waller factor and static vs. thermal disorder. X-ray Absorption Fine Structure contains vital information about the surrounding system of an absorbing atom including crystal structure, bond distances and coordination number. It is crucial that we understand all processes that may affect the measured XAFS spectra. The aim of this study is to investigate thermal effects and quantify thermal and static disorder [1]. The XERT is an experimental technique developed by our group, capable of measuring X-ray mass attenuation coefficients on an absolute scale with accuracies down to 0.02% [2]. This study has taken crucial elements from the XERT and applied them to complex experimental systems. This includes, but is not limited to high accuracy energy calibration [3], quantification and correction of beam harmonics and fluorescence. Our robust technique allows us to take the high accuracy data required to determine fundamental structural and crystallographic properties. These developments give great insight into our understanding of more complex systems such as organometallic molecules and biological systems.

[1] J.D. Bourke, C.T. Chantler and C. Witte, *Phys.Lett.A*, 360(6), 702-706 (2007), [2] M.D. de Jonge, C.Q. Tran, C.T. Chantler, et al.i, *Phys.Rev.A*, 71(3), 032702 (2005), [3] L.J. Tantau, M.T. Islam, A.T. Payne, et al., *Rad.Phys.Chem*, 95, 73-74 (2014)



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