



Aalborg Universitet

AALBORG UNIVERSITY
DENMARK

Vibrational Properties of Nanograins and Interfaces in Nanocrystalline Materials

Stankov, S.; Yue, Yuanzheng; Miglierini, M.; Sepiol, B.; Sergueev, I.; Chumakov, A. I.; Hu, L.; Svec, P.; Ruffer, R.

Publication date:
2008

Document Version
Publisher's PDF, also known as Version of record

[Link to publication from Aalborg University](#)

Citation for published version (APA):

Stankov, S., Yue, Y., Miglierini, M., Sepiol, B., Sergueev, I., Chumakov, A. I., Hu, L., Svec, P., & Ruffer, R. (2008). *Vibrational Properties of Nanograins and Interfaces in Nanocrystalline Materials*. Abstract from 9th International Conference on Nanostructured Materials, Rio de Janeiro, Brazil , .

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- ? Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- ? You may not further distribute the material or use it for any profit-making activity or commercial gain
- ? You may freely distribute the URL identifying the publication in the public portal ?

Take down policy

If you believe that this document breaches copyright please contact us at vbn@aub.aau.dk providing details, and we will remove access to the work immediately and investigate your claim.

Vibrational Properties of Nanograins and Interfaces in Nanocrystalline Materials

S. Stankov¹, Y. Z. Yue^{2,3}, M. Miglierini⁴, B. Sepiol⁵, I. Sergueev¹, A. I. Chumakov¹, L. Hu^{2,3}, P. Svec⁶, and R. Rüffer¹

¹*European Synchrotron Radiation Facility, BP220, 38043 Grenoble, France*

²*Section of Chemistry, Aalborg University, 9000 Aalborg, Denmark*

³*Key Laboratory of Liquid Structure and Heredity of Materials, Shandong University, 250061 Jinan, China*

⁴*Department of Nuclear Physics and Technology, Slovak University of Technology, 81219 Bratislava, Slovakia*

⁵*Fakultät für Physik, Universität Wien, 1090 Vienna, Austria*

⁶*Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, Slovakia*

The vibrational dynamics of nanocrystalline $\text{Fe}_{90}\text{Zr}_7\text{B}_3$ was studied at various phases of crystallization by ^{57}Fe nuclear inelastic scattering of synchrotron radiation. The average sizes of the nanograins were determined by the Rietveld refinement of the X-ray diffractograms, while the volume fraction of the interfaces was obtained from the conversion electron Mössbauer spectra by applying a well established fitting model [1, 2]. The density of phonon states (DOS) of the nanograins was separated from the DOS of the interfaces for a wide range of grain sizes and interface thicknesses. Surprisingly, DOS of the interior and the surface of the nanograins do not vary with the grain size and closely resembles that of the bulk material down to 2 nm. The anomalous enhancement of the phonon states at low and high energies observed in the DOS of the nanocrystalline materials [3], originates entirely from the vibrational modes of the interface exhibiting a characteristic DOS of a significantly disordered matter. The low energy enhancement of phonon states scales linearly to the volume fraction of the interfaces and perfectly obeys the Debye law for the interface thickness below 0.5 nm.

The obtained results give an unambiguous evidence that the anomalous dynamics and thermodynamics of nanocrystalline solids originate from the disordered interfaces, while thermodynamical properties of the nanograins are essentially bulklike and to a large extent size-independent. These findings are of significant importance for the continuously increasing number of technological applications of the nanocrystalline materials. In particular they reveal that tailoring of certain thermo-elastic properties requires to control precisely the volume fraction of the nanograins rather than of their sizes.

[1] M. Miglierini, and J. M. Greneche, *J. Phys.: Condens. Matter*, **9**, 2303 (1997).

[2] M. Miglierini, and J. M. Greneche, *J. Phys.: Condens. Matter*, **9**, 2321 (1997).

[3] B. Fultz, C. C. Ahn, E. E. Alp, W. Sturhahn, T. S. Toellner, *Phys. Rev. Lett.* **79**, 937 (1997).

Corresponding author: Svetoslav Stankov, stankov@esrf.fr

Keywords: nanocrystalline $\text{Fe}_{90}\text{Zr}_7\text{B}_3$, vibrational density of states, nuclear inelastic scattering