Structural studies of ScFe and PdSi nanoglasses using SAXS and XRD

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Nanoglasses are produced from amorphous nanoparticles of an alloy by inert gas condensation.[1] We studied the effect of thermal annealing to ScFe and PdSi nanoglasses at beamlines B1, C and BW5. Small-angle X-ray scattering (SAXS) gave information about the nm-scale structure of the interface areas between the nanoparticles in the nanoglasses. High-energy X-ray diffraction (XRD) gave information on the coordination of the atoms inside the nanoglasses.

In the experiments made at B1, we found that, unlike predicted by Monte Carlo simulations, heat treatment of ScFe nanoglass does not easily lead to fully homogeneous structure of the alloy. By fitting Debye–Bueche random phase model to the SAXS data, we could follow the development of a characteristic correlation length, which tells us about the size of interface areas between nanoparticles in the nanoglass. In addition, the mean square fluctuation in electron density can be determined and thus one can observe if and when the density difference between the interfaces and the nanoparticles vanishes and the alloy becomes fully homogeneous. It was found that such fully homogeneous nanoglass was experimentally not achieved for several ScFe nanoglass samples, possibly because of nanophase separation of Sc. [2] Figure 1 shows the results for one such annealing of a ScFe nanoglass. Although the electron density difference between the nanoparticles and the interfaces decreases, it does not reach zero. Meanwhile, the correlation length increases during annealing, indicating growth of the interface regions. Similar measurements were made for PdSi nanoglasses.

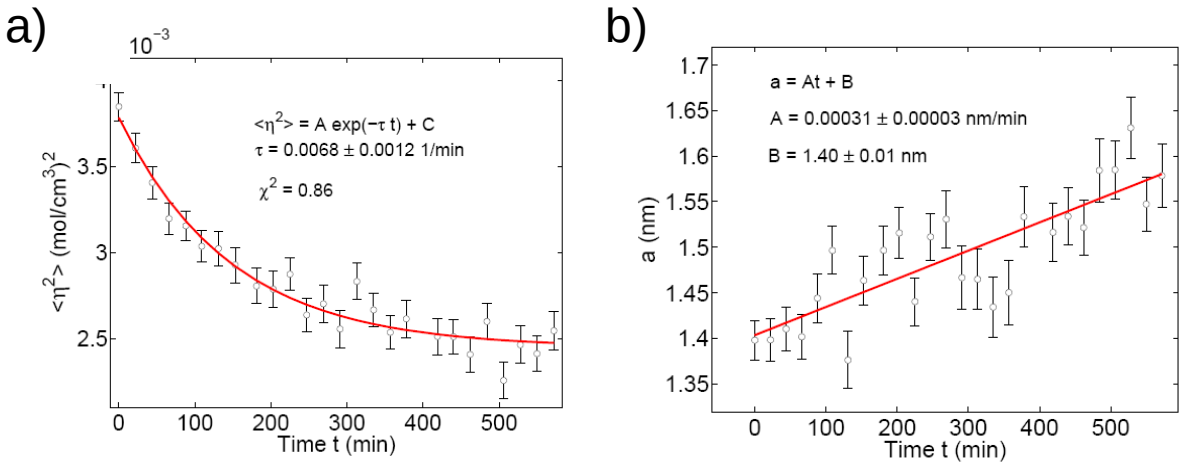

Figure 1: a) Change in the mean square fluctuation in electron density as a function of time in one ScFe nanoglass alloys during annealing at 200 °C. b) Change in the correlation length as a function of time for the same sample.

In XRD, the structure factor (not shown here) exhibit broad and diffuse maximum appearing at q=2.55 Å^{-1} with slightly varying oscillations which tend to vanish with increasing wave vector q. In order to observe very fine structural changes occurring in the sample during constant rate (5 °C/min) annealing up to 230 °C, the difference plot was produced from calculated structure factors $S(q)$. Figure 2a shows evolution of the difference structure factor, $\Delta S(q)_T = S(q)_T - S(q)_{T0}$. One can clearly observe that around 140 °C positive and relatively sharp peaks appear and thus indicate early stages of the ongoing crystallization. It should be noted here that these peaks are rather small

compared with the maximum intensity observed in diffraction patterns. However, using highly intense photon beam in combination with two-dimensional detector results in excellent signal-to-noise ratio and thus allowing an observation of very fine structural features, which would be otherwise buried in the noise. All structure factors *S(q)* were Fourier transformed in order to get corresponding real space pair distribution functions, *G(r)*. Mean atomic density ρ_0 and coordination number CN for the first coordination shell obtained form pair distribution functions are shown in Fig.2b. One can observe that mean atomic density initially decreases with increasing the temperature whereas coordination number remains within experimental uncertainty constant. After reaching 120 °C both parameters increase with increasing temperature. Such an increase could be correlated with structural modifications associated with the early stages of the crystallization.

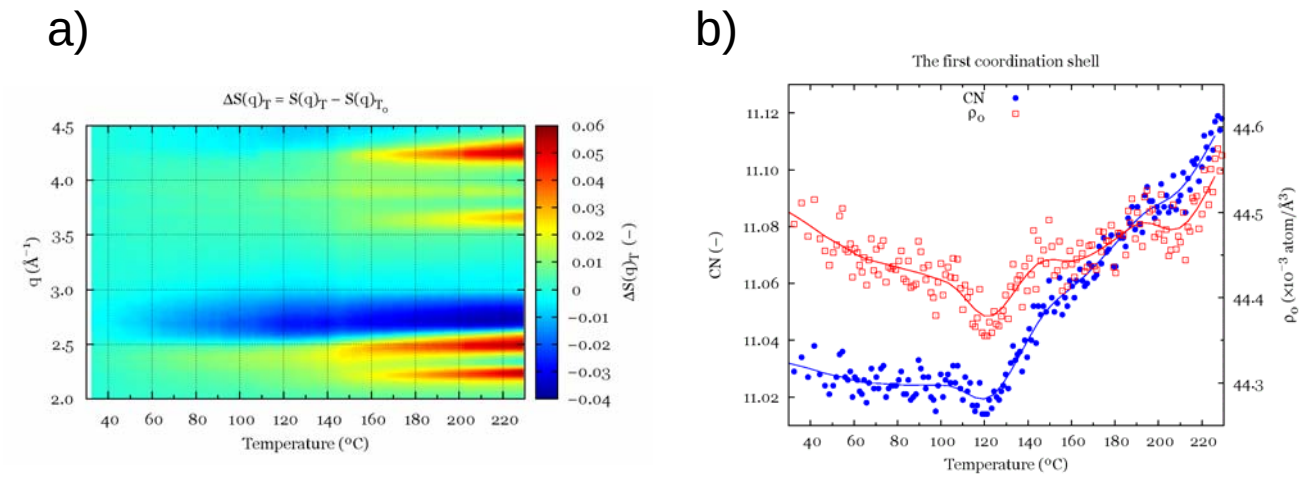

Figure 2: a) Temperature evolution of the difference structure factor $\Delta S(q)_T = S(q)_T - S(q)_{T0}$. b) Mean atomic density ρ_0 (red open squares) and coordination number CN (blue solid circles) as a function of temperature. Full lines (Bezier splines) are guides for eyes.

References

[1] H. Gleiter, MRS Bulletin **34**, 456 (2009).

[2] J. X. Fang, U. Vainio, W. Puff, R. Würschum, D. Wang, M. Ghafari, H. Hahn, H. Gleiter, manuscript in preparation.