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DETERMINATION OF PARTIAL STRUCTURE FACTORS USING A THIRD GENERATION SYNCHROTRON SOURCE: In-Se AMORPHOUS FILMS

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In the structural studies of non-crystalline materials such as glasses, amorphous films and alloys, liquids and other disordered materials there is much interest in maximizing the amount of information about such systems. The structure of non-crystalline materials is usefully expressed in terms of the pair distribution function, which is obtained from the structure factors via the sine Fourier transform. When a sample contain n atomic species there are $n(n\text{-}1)/2$ distinct partial structure factors. It should be noted that knowledge of the partial structure factors is the most complete information that can be obtained from a scattering experiment for non-crystalline materials [1-3].

The resonant changes in the complex X-ray atomic scattering factors defined as

$$f(K,E) = f_0(K) + f'(E) + if''(E)$$

can be used to vary the weights $W_{jk}(K,E)$ of the individual partial structure factors $S_{jk}(K)$ to the total structure factors $S(K,E)$

$$S(K,E) = \sum_{j=1}^{n}\sum_{k=1}^{n} W_{jk}(K,E) S_{jk}(K),$$

where $K=4\pi\sin\theta/\lambda$, λ is the wavelength, E is the energy of the incident photons,

$$W_{jk}(K,E) = c_j c_k \,\mathrm{Re}\frac{f_j(K,E) f_k(K,E)}{< f(K,E) >^2},$$

$$< f >= \left| \sum_{j=1}^{n} c_j f_j \right|^2$$

and c_j indicates the concentration of the jth atomic species.

Anomalous X-ray scattering has been used to determine the partial structure factors for vacuum evaporated In-Se films containing 50 and 66 at.% Se. The X-ray scattering data were collected at the European Synchrotron Radiation Facility (ESRF, Grenoble, France) on the ID01 beam line (anomalous X-ray scattering) using incident photon energies tuned exactly at the Se and In absorption K-edges (12653 and 27950 eV, respectively) and below the edges at 11800 and 27000 eV. The edge positions were determined experimentally for each sample from the fluorescence EXAFS scans. The values of the real and imaginary parts of the atomic scattering factors f' and f'' for the energies at the Se and In edges were calculated from previously recorded EXAFS data using the Kramers-Kronig relationship within the frame of the optical theorem [4]

$$f''(E) = \frac{mcE}{4\pi\hbar e^2}\mu(E)$$

$$f'(E) = \frac{2}{\pi} VP\int_0^{\infty} \frac{E' f''(E)}{E^2 - E'^2} dE' + \Delta f',$$

in which m and e indicate the mass and charge of an electron, c is the light velocity, $\mu(E)$ is the linear absorption coefficient and VP denotes the Cauchy principal value of the integral.

From the determined structure factors the partial pair distribution functions $4\pi r^2\rho_{jk}(r)$ were computed as follows

$$d_{jk}(r) = \frac{2}{\pi}\int_0^{K_{\max}} K[S(K)-1]\frac{\sin(\pi K/K_{\max})}{\pi K/K_{\max}}\sin(Kr)dK$$

$$4\pi r^2\rho_{jk}(r) = c_j\left[4\pi r^2\rho_0 + r d_{jk}(r)\right],$$

where ρ_0 is the macroscopic number density. The availability of the intense radiation source as the third generation synchrotron has made it possible to obtain reliable data much better conditioned when compared with previously obtained results. The obtained results show that both investigated amorphous films exhibit certain degree of chemical disorder within the model based on crystalline InSe. The present findings are compared with the results of similar studies carried out for the amorphous Cd-As amorphous films using a second generation source as well as with the isotopic substitution technique developed for neutron scattering.

References

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