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MODELING OF THE INTERFERENCE OF ELECTRON WAVES SCATTERED ON THE AMORPHOUS MATERIALS

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The RDF method use to analyze of amorphous structure the formal features of difference $4\pi r^2[\rho(r) - \rho_0]$, which has no clear physical content. It is mathematically defined from the structure factor or intensity of coherent scattering electrons. This uses a number of assumptions and approximations, each of which makes the end result in some errors. In the same experiment diffraction pattern of amorphous material formed as a result of the imposition of certain interference functions from the fixed inter atomic distances disordered atomic network. Therefore, analysis electron diffraction patterns preferably also hold directly on real structural parameters this network.

In establishing these parameters all atomic network conventionally divided into separate averages of the real structure, coordination sphere. It believes that each coordination sphere of atoms is the origin of a certain averaged distances r_k called the coordination sphere radius. Each coordination sphere is also attributed to the corresponding average coordination number Z_k, which determines the average number of atoms that are in this coordination sphere. Ideally believe that all atoms of this coordination sphere have the same interatomic distance equal to r_k. For such an ideal model of each k-coordination sphere in the structure factor gives a contribution in the form of the Debby interference function $i_k(s)$:

$$i_k(s) = Z_k \sin(sr_k)/(sr_k).$$

In the real situation is complicated by the presence in networks of interatomic distances fluctuations. This fact can be given, as if each k-coordination sphere as separate in some way selected radial distribution function of atomic density $\rho_k(r)$. In this approximation can be written:

$$4\pi r^2 \rho_k(r) = \frac{Z_k}{\sqrt{2\pi\sigma_k^2}} \exp\left[-\frac{(r-r_k)^2}{2\sigma_k^2}\right],$$

where σ_k^2 - dispersion of interatomic distances distribution of k-coordination sphere. Natural question arises: how interatomic distances fluctuation affects of interference function? To answer this question we have calculated interference functions of local areas of real atomic network of amorphous silicon films. Our results show that experimental studies of atomic parameters of amorphous network can be based on physically well-defined radial distribution function of atomic density $\rho(r)$. This should set the differences in the regularities of interference functions of local areas for cases describing atomic network by functions $4\pi r^2[\rho(r) - \rho_0]$ and $4\pi r^2\rho(r)$. Such analysis was making by computer simulation using the conventional theoretical approaches.