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Structural refinement of amorphous alloy nanovolumes using RDF analysis

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As structural components of devices and materials diminish in size, there is increasing interest in developing capabilities to analyse amorphous nano-volumes. The technique of electron energy selected reduced density function (RDF) analysis is one of the few techniques with this capability. Originally developed to study thin films [1], the technique has been recently extended to volumes approaching 1 nm in width [2]. This allows local variations in structural order to be studied, for example in intergranular films, amorphised volumes (e.g. in DVDs) and barrier layers. In extending the RDF technique to the nanoscale, a number of important experimental problems had to be overcome, including the incident probe convergence and the effect of electron beam coherence on the interpretation of the data [3-4].

While the resulting data, in the form of G(r) can be interpreted straightforwardly for elemental systems (e.g. a-C, a-Si), the interpretation is less straight forward for alloys. In the case of a binary alloy, we can obtain the structure factor *S(*q) directly from the diffraction pattern I(q) if we know the concentrations c_i of the two elements and their scattering factors f_i. W(r), the Fourier transform of S(q) – 1, can then be expressed as

$$W(r) = \sum_i \sum_j A_{ij}(r) \otimes W_{ij}(r) \qquad (1)$$

where $A_{ij}(r)$ is the Fourier transform of α_{ij} and $\alpha_{ij} = c_i c_j f_i f_j / [[c_1 f_1 + c_2 f_2]^2$

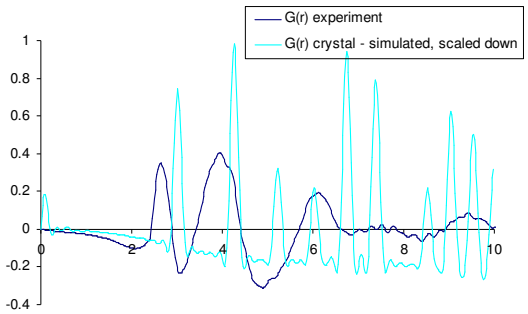
W_{ij} (r) is then directly related to the density of atoms i around j.

If $\alpha_{ij}(q)$ is slowly varying with q (the scattering vector), then W(r) can be treated as the weighted sum of the partial $W_{ij}(r)$ (weighted by α_{ij} (0)). To the extent that α_{ij} is not slowly varying, this approach is an approximation.

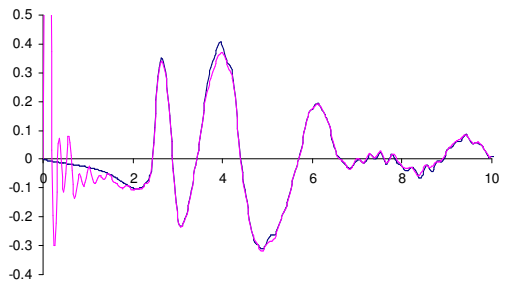
An alternative approach is to use W(r) as a data set against which to refine the W'(r) obtained from a model structure. W'(r) can be obtained by calculating I'(q) from the model, and then refining the model (e.g. Monte Carlo refinement) to achieve W'(r) = W(r). The resulting model will not be unique, and constraints must be applied (e.g. energy constraints, restricting atomic displacements) if unphysical models are to be avoided.

It is to be noted that it is not correct to obtain the partial distribution functions from within the model to compare with W'(r), as equation 1 demonstrates.

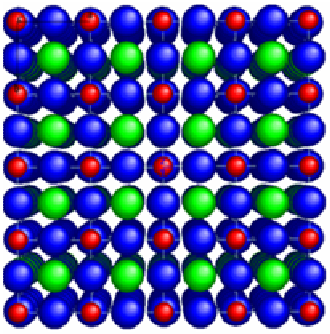
An example of refining W(r) against W'(r) is shown in figure 1, obtained from thin film $Ge_2Sb_2Te_5$ (candidate material for fast switching DVDs).

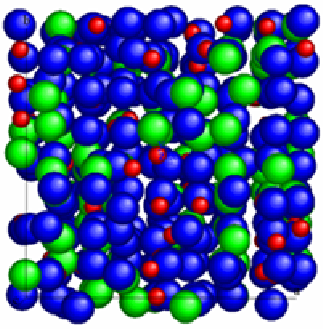


W'(r) of the NaCl type crystal (structure shown below) in comparison with the experimental data recorded from an amorphous $Ge_2Sb_2Te_5$ layer. r is given in Angstrom and the units on the second axis (W(r)) are arbitrary.



Experimental W(r) and the refined W'(r) when taking a NaCl type crystal as a starting model. r is given in Angstrom and the units on the second axis are arbitrary. The resulting (refined) amorphous structure is shown below.





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