

# What Stabilizes the Intermediate Structure of an Amorphous Alloy?

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Structure determines dynamics. More specifically, stability determines dynamics and structure represents our way of understanding stability. While these observations represent all too obvious truisms in the study of crystalline solids, they are maxims rarely applied in amorphous solids. The difficulties are twofold - we often lack useful descriptions of amorphous structure, and we need a rationale that relates structure and stability. The goal of this paper is address both difficulties in the context of a well characterised model of a binary metal-metalloid glass forming alloy. To this end we present the results of simulation studies of a model binary alloy based on the Ni-P system in which we characterize and explain the local coordination structure, the intermediate structure associated with the packing of these coordination polyhedra, the relationship between the structure and the potential energy landscape of this glass former and the thermal stability of the various structural elements of this model amorphous solid.

The model system is consists of a binary mixture of particles interacting via Lennard-Jones potentials. The potential parameters, due to Kob and Andersen [1], include a substantially stronger attraction between the smaller species B (the solute) and A (the solvent) than between B and B. This preference for AB interactions generates chemical ordering in the low temperature liquid characterised by the B particles being coordinated solely by A particles. Intermediate structure refers to the organisation of these solute coordination polyhedra. Previously [2] we have shown that the solute-solute radial distribution function  $g_{BB}(r)$  describes the length scales arising from this intermediate structure. This distribution of length scales can be resolved into solute-solute pairs that share 4, 3, 2 or 1 solvent neighbours. We shall refer to such pairs as being  $B^nA$  bonds where n equals the number of shared A's. These bonds refer to how two adjacent solute coordination polyhedra are connected with an  $B^3A$  bond corresponding to a shared triangular face, a  $B^2A$  bond referring to a shared edge and a  $B^1A$  bond, a shared vertex.

In this paper we extend this analysis. First, we examine the spatial distribution of the  $B^3A$  bonds in both the amorphous state and in crystals of the  $A_3B$  alloy and find that there appears to be no strong correlations between these bonds in the amorphous system beyond a pairwise correlation involving two bonds sharing a common solute. We show that the distribution of angles between these bond pairs is sharply structured (see Figure 1) and that this structure can be attributed to the

organisation of B particles about the solvent A .

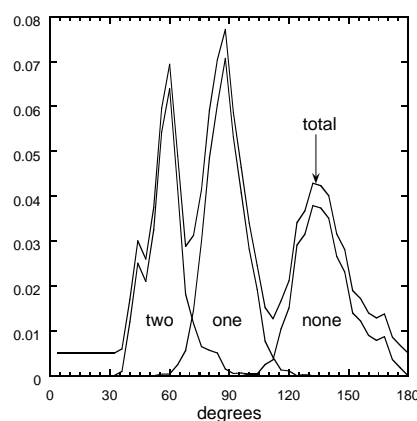


Figure 1. The distribution of angles between  $B^3A$  bonds in an amorphous  $A_3B$  mixture at  $T = 0$ . Note that the sharp peaks about  $60^\circ$ ,  $90^\circ$  and  $135^\circ$  can be directly associated with pairs of  $B^3A$  bonds with two, one or no A neighbours common to all three B particles.

Next, we examine the energetics of the various B centered and A centered coordination structures and find that they are generally close to their minimum energy values. This observation supports the proposition that the geometric frustration arising due to the presence of coordination polyhedra that cannot fill space is relaxed in an alloy by compositional variations instead of by strain as is found in one component glass models [3].

Finally, we compare the amplitude of particle displacements associated with different coordination structures as a function of temperature.

## References

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