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Local Structural Distortions in Quenched Au-Cu Alloys

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Abstract: Disordered alloys Au_xCu_{1-x} prepared by melt spinning method were analyzed by XAFS taken at 80 K. Local atomic structure around Au and Cu atoms was measured and strong deviations from perfect *fcc* structure were obtained resulting from the size disparity between Au and Cu atoms. A sharp asymmetry was found between the shorter (Cu-Cu) and the longer (Au-Au) nearest neighbor bond lengths. Average first nearest neighbor distance was found greater than obtained using linear interpolation of the pure components. Results on Debye-Waller factors showed strong concentration dependence for the Cu-Cu bond, suggesting the loosening of contact between these atoms when the concentration of Au increases.

As a result of our extended XAFS study of mixed crystals with atomic size mismatch [1] a basic asymmetry between larger and smaller atoms' behavior has been revealed. The XAFS measurement allows to distinguish an interatomic distance within a particular atomic pair from an interplanar spacing as ascertained by diffraction. Since all the cubic crystals were found to have non-collinear bond structure (*buckling* [2]), their average interatomic distances, weighted with concentration, had to be always greater than the interplanar spacing. We present results of the XAFS analysis of the quenched Au_xCu_{1-x} alloys at 80 K where the random distribution of Au and Cu atoms in the average *fcc* lattice was accompanied by bond buckling, peaked in the midst of the concentration range. Contact loosening between Cu-Cu atoms increased with growing x , while Au-Au and Au-Cu atoms kept in touch at all concentrations.

Metallic alloys Au_xCu_{1-x} ($x = 0.06, 0.35, 0.56, 0.80, 0.96$) were prepared by melt spinning method in the Technion, Haifa, Israel. The cooling rate was approximately 10^5 K/sec, to ensure the homogeneity of the samples. The homogeneity was verified by X-ray diffraction and no trace of phase separation was observed. The XAFS measurements of Au L_3 - and Cu K - edges were performed on beamline X11A at NSLS at 80 K.

XAFS signals were analyzed by the UWXAFS software [3]. Theoretical scattering amplitudes and phases were generated using the FEFF6 code [4] for the *fcc* crystal structure model. XAFS analysis was performed concurrently for two edges for each concentration while fitting the FEFF6 theory to data. Changes occurring in the local structure were parameterized in the fit process as corrections to interatomic distances. Mean square deviations of the first nearest neighbor (1NN) bond lengths σ^2 (XAFS Debye-Waller factors) were varied independently for each bond. Parameters of the Au-Cu bonds were constrained in the fit to be the same as seen from each edge. Local composition y was allowed to vary in order to account for possible short range ordering of like or unlike atoms.

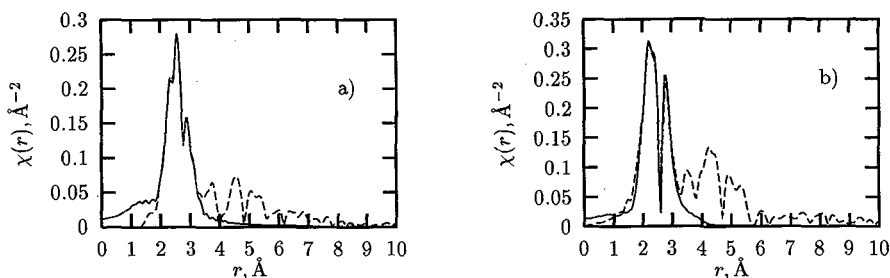


Figure 1: Fourier transforms of the k -weighted XAFS spectra simultaneously fitted with FEFF6 theory (solid) to the data (dash) of $Au_{0.8}Cu_{0.2}$ at 80 K for a) Au L_3 and b) Cu K edges.

Fits to the data are shown in Fig. 1. Local compositions y were found to be equal to the bulk concentrations x of the alloys, indicating absolutely random substitution of atoms. 1NN distances (Fig. 2 a)) show clear asymmetry with respect to the linear interpolation of the pure components, similar to what was obtained previously for the mixed salts $RbBr_xCl_{1-x}$ [1]. As discussed in Ref. [1], such asymmetry is a consequence of the local static distortions in the lattice caused by the asymmetry of the repulsive and attraction branches of the interatomic potential. While the

bond buckling would result in the average 1NN distance (d_{XAFS}) being always greater than the average interplanar spacing d_{XRD} , measured by x-ray diffraction (XRD), our result for the (d_{XAFS}) (Fig. 2 a), crosses) almost coincides with the experimental XRD data at the same temperature (the XRD data at 80 K were obtained by using the room temperature data [5] and correcting by thermal contraction [6] to 80 K). This nonlinear dependence of the d_{XRD} with x is consistent with a lattice parameter increase due to the positive tendency to clustering of like atoms in alloys [5], i. e. prepared with insufficiently fast quenching rates and, therefore, non-random. As indicated in Ref. [6], the positive tendency to clustering is just the case for the disordered Au-Cu alloys obtained by quenching in water. In our case the randomness of the atomic distribution was assured by the fast quenching rate (10^5 K/sec), and, therefore, to illustrate the asymmetry between the repulsion and attraction (as in $\text{RbBr}_x\text{Cl}_{1-x}$ [1]) the mean 1NN distance, (d_{XAFS}), should be compared with the straight line connecting the pure components and corresponding to the d_{XRD} of the absolutely random alloy.

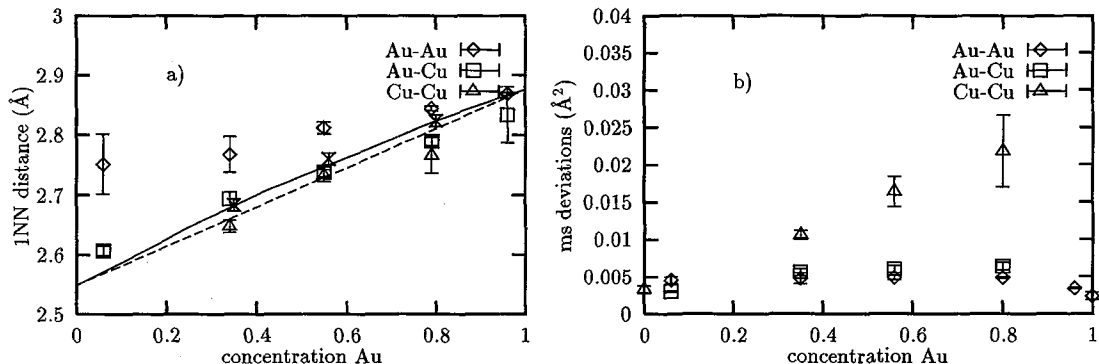


Figure 2: a) 1NN distances as determined by x-ray diffraction (solid), linearly interpolated with concentration (dash), and measured by XAFS (symbols). Concentration-weighted average 1NN distances obtained with XAFS and shifted for clarity are shown by crosses. b) Mean square deviations of the 1NN bond lengths.

The different tendency of Au-Au and Cu-Cu bond lengths to change with concentration was confirmed in the measurements of the Debye-Waller factors (Fig. 2). Consistent with a relatively small decrease in Au-Au bond length with respect to its value in pure Au, the σ^2 of this bond does not change strongly with x either. This is in contrast with the Cu-Cu bonds which have a drastic increase of σ^2 with x , consistent with the Cu-Cu distance expansion to be greater than the Au-Au contraction (with respect to the pure metal values). These results indicate that the small Cu atoms become loosened in the Au matrix at large enough x ($x > 0.35$), and the Cu-Cu 1NN pairs are losing contact, while Cu-Au and Au-Au 1NN pairs remain in contact at all concentrations.

In conclusion, our results show that the rapidly quenched alloys $\text{Au}_x\text{Cu}_{1-x}$ are completely random at all x . Locally, the structure is buckled about the perfect fcc lattice with the equilibrium positions of Cu atoms to be most distorted. The buckling is the greatest in the midst of the concentration range, where the difference between the average nearest neighbor distance and the interplanar spacing in the completely random alloy is maximized.

Acknowledgments

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