Comment on ''Anomalous Temperature Dependence of the X-Ray Diffuse Scattering Intensity of Cu_3Au"

Reichert, Moss, and Liang (RML) have recently reported [1] the observation of an *increase* in the splitting of the short-range-order (SRO) diffuse scattering peaks in disordered Cu_3Au alloys as the temperature was raised above the order-disorder transition. The major point of their work was that this temperature-dependent increase was "anomalous" and "unexpected" and that "currently, there are no three-dimensional first-principles theories which are capable of explaining such a temperature-dependent fine-structure of the diffuse scattering." RML further noted that the standard method of Monte Carlo (MC) simulations of local density approximation (LDA)-derived first-principles alloy Hamiltonians, applied by Lu, Laks, Wei, and Zunger (LLWZ) to a different system—disordered Cu_3Pd alloys [2], "indicate that the splitting of the diffuse peak is *decreasing* with increasing temperature for $Cu_{0.7}Pd_{0.3}$ . . . in contrast with our finding in Cu_3Au." Inspection of the paper of LLWZ [2] shows that the temperature dependence of the SRO splitting was simply not calculated or even mentioned there. Thus, RML's characterization of the results of Ref. [2] is incorrect. And, since Cu_3Pd (for which there are no T-dependent experiments on equilibrated samples) is different from Cu_3Au, we undertook T-dependent SRO calculations here. We find that the T-dependent splitting in Cu_3Au is trivial consequence of the *configurational* entropy, which is properly included in standard three-dimensional first-principles alloy theories [2].

Figure 1 shows the calculated SRO intensity in disordered Cu_3Pd and Cu