Narasimhan and Jarić Reply: In Ref. 1, we suggested that periodic (rational) approximants could compete with our icosahedral quasiperiodic structure, and should be examined. Indeed, Smith and Rabson[2] report that one of the approximants[3] has significantly lower energy (zero-temperature, zero-pressure enthalpy), and they conjecture that icosahedral quasiperiodic ground states are most likely limited to two-or-more-component compounds.

Let us reiterate that our icosahedral structure was optimized for the Lennard-Jones (LJ) potential, *not* the square-well (SW) potential. Since the LJ potential has a sharp minimum and decays very rapidly, this effectively means that the structure was optimized to maximize the frequency of the *shortest* bond. However, at the well width of 0.71σ, there are at least five coordination shells that contribute to the cohesive energy, and it is necessary to maximize the *total* effective coordination.[2] Thus the energy[1] of -13.5ϵ is at best an upper bound; icosahedral quasiperiodic structures with lower energy certainly exist. It is not yet known if a full optimization will give energies lower than for the rational approximant mentioned above.

We note that the packing fractions are optimized by domains that are polyhedra with planar faces with icosahedral symmetry. In particular, for si structures the optimal domain, related to the second peak in Fig. 2 of Ref. 1, can be shown to be a certain truncated dodecahedron, obtained by drawing planes normal to the fivefold directions, at a distance $R_f=0.500a$, and planes normal to the twofold directions at a distance $R_e=0.526a$, from the center. The length of the shortest bond is $R_s=2.384a$, the packing fraction is $\phi=0.574$, and the SW energy is -6.8ϵ in the range $0.70 \leq w/\sigma \leq 0.73$. The other high-density structure, related to the first peak in Fig. 2 of Ref. 1, has a regular icosahedron for the domain.[4] The distance to the midpoint of a face is $R_f=1.192a$, the shortest bond length $R_s=1.000a$, the packing fraction $\phi=0.56$, and the SW energy of -13.4ϵ. These polyhedra maximize the frequency of the shortest bond. Since the cohesive energy for the SW interaction is controlled solely by the packing geometry, the optimal domains will again be polyhedra, possibly with a complex topology.

The trend towards structures with larger unit cells as the well width increases should be noted. While it seems likely that the ground state in the case of a strictly finite-range potential is periodic, real metallic potentials decay relatively slowly and show Friedel oscillations. If the competing periodic structures are rational approximants, the set of bond lengths that appear in the structure forms a subset of the possible bond lengths in the quasiperiodic structure. The latter form a denser set (though this difference is noticeable only at large distances). In other words, there are more coordination shells within a given distance in the quasiperiodic structure. Thus, the tail of the potential may serve to stabilize the icosahedral phase. If the competing periodic structure is not a rational approximant, then the bond lengths in the two cases are not related in general. Depending on where the maxima in the potential fall, one or the other structure will be suppressed.

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