

Yan, Pennycook, and Pang Reply: It was not our intent to redefine or extend the definition of the structural vacancy. In our Letter [1] we specifically point out that the pairs of closely spaced columns observed in our Z-contrast images, at 1.4 Å separation, are too close to be fully occupied (we quote, "It is clearly not possible for each column within a pair to be fully occupied."). We suggested that these columns were half-occupied and that the two columns could equally well be regarded as a single buckled column (see Fig. 1). Coddens objects to our referring to these half-occupied column pairs as columnar vacancies [2]. It is right that if two adjacent sites cannot be filled, then clearly the unoccupied site cannot be *exactly* equivalent to a *regular* structural vacancy. However, it is clear that the half-occupied columns *do* have some vacancy *character* since they can be regarded as a splitting of a single fully occupied column. This results in a significant unoccupied volume, though not so large as a true structural vacancy, and must represent a more stable site for a diffusing transition metal atom than the interstitial location it would otherwise need to occupy. Therefore, we would expect significant changes in the activation barrier for diffusion along the *c* axis, but only through these particular sites, which act as "pipes" within the clusters. We also point out the role of such sites in mediating phason flips. Because such sites occur only in *specific* columns in the 2 nm cluster, we feel that their columnar nature is an important feature, which is the reason we refer to them as columnar vacancies.

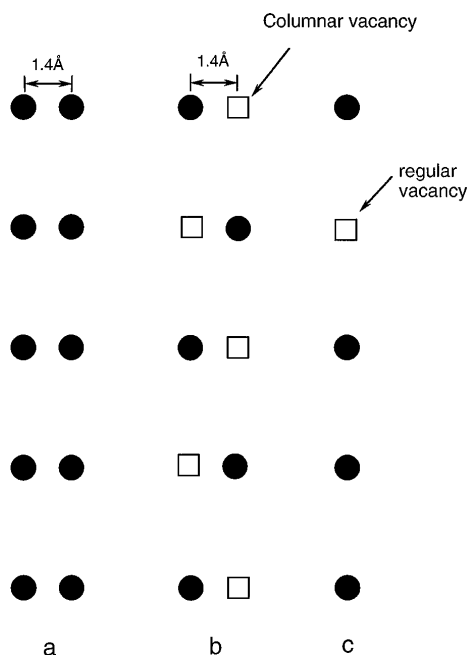


FIG. 1. Schematic showing (a) two closely spaced columns with full occupancy; (b) columnar arrangement of vacancies consistent with image intensities. Although these sites have vacancy character, the nearby filled site means they are not equivalent to the structural vacancy of an isolated column (c).

Perhaps it is worth mentioning that very similar features have been seen previously in Z-contrast images of grain boundaries in SrTiO₃. The dislocation cores comprising <100> tilt grain boundaries (both symmetric grain boundaries and the quasiperiodic asymmetric boundaries) all show closely spaced pairs of columns, either on the Ti or Sr sublattice [3,4]. These column pairs are also too close for full occupancy, and were referred to as half-columns. They cannot be regarded as structural vacancies for the same reason; they cannot be filled. But most certainly they will mediate pipe diffusion along the core. In the case of the quasicrystal we recognized the same features, although not associated with dislocation cores but with specific rings in the structure.

Columnar vacancies will clearly have important implications for mass transport, as well as for phonon and electron transport properties. In fact, the tendency for closely spaced sites to mediate rapid diffusion and phason flips in quasicrystals has already been pointed out in the molecular dynamics studies of Gahler and Roth [5], which we cited in our Letter. These authors referred to such sites as half-vacancies. They did not predict the columnar arrangement, but they did find strong columnar characteristics. Diffusion occurred predominantly along the *c* axis, but diffusing species kept mostly within one particular closely spaced pair of columns. Again the term columnar vacancy seems appropriate.

Finally, we mention that we observed similar columnar vacancies on the Al sublattice, again in a specific ring in the cluster. Therefore localized, anisotropic, columnar properties are expected on both sublattices.

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