Schiller *et al.* Reply: Contrary to what is stated in the preceding Comment by Bendounan *et al.* [1], we were perfectly aware that the 1 ML Ag moiré analyzed in Ref. [2] has the same triangular dislocation lattice as the one presented in Ref. [1]. In Ref. [2] one can literally read that the preparation procedure "leads to a triangular structure with Cu vacancies and dislocation loops in the substrate." Most important, Bendounan *et al.* discuss the transition from the 9×9 pattern without triangular dislocations to the $\sim 9.5 \times 9.5$ pattern with triangles, which is not the key point in Ref. [2]. The issue is why the out-of-registry $\sim 9.5 \times 9.5$ reconstruction (with triangles) is preferred for 1 ML instead of the registry 9×9, characteristic of 2 ML. This is particularly remarkable, since, assuming a Ag/Cu coincidence lattice, the 9×9 has lower Ag overlayer compression. What we claim is that, at the temperature at which triangular misfit dislocations form ($T >$ 200 K), the out-of-registry pattern is due to Fermi surface (FS) nesting at $\bar{M}$. Otherwise, in-registry phases appear as in 2 ML [2].

The data shown by Bendounan *et al.* for the lattice of triangles are entirely consistent with those presented in Ref. [2], and with the measurements performed at 180 and 300 K, which are displayed in Fig. 1. Here we prove that differences are only due to the measuring temperature, and by no means due to a "lack of precision in sample orientation," as wrongly estimated by Bendounan *et al.* [3]. One can observe the same temperature-dependent rigid shift of the surface band as in Ag(111) or Cu(111) (40–45 meV from 40 to 300 K [4]), which is due to changes in atomic lattice constants. The band bottom at $\bar{\Gamma}$ shifts from $E_0 = -241$ meV at 40 K [1] to $E_0 = -217$ meV at 180 K and to $E_0 = -197$ meV at 300 K. As a consequence, the upper band gap edge at $\bar{M}$ shifts from $E_{\bar{M}} = 2 \pm 4$ meV at 40 K [5] to $E_{\bar{M}} = 35 \pm 5$ meV at 300 K. Thus, the $\bar{M}$ gap is present within a very wide range above and below the moiré triangular structure transition at 200–250 K.

Once the triangular dislocation lattice is formed, strong temperature-induced band structure changes such as those of Fig. 1(a) are not likely to be balanced by changes in the superlattice, since this involves a major substrate disruption. Thus, any possible structural or electronic energy interplay scenario, i.e., a charge density wave (CDW)-like state, must be considered only at temperatures close to 200 K. In Fig. 1(b) we show the two-dimensional (2D) FS measured at 180 K. We observe nesting over a large portion of the 2D FS, with small hole pockets at $\bar{K}$. Such a FS is similar to that of Bi(111) [6], for which a 2D CDW-like state is claimed. Figure 1(b) also includes the FS obtained from a model calculation that fits experimental surface bands along $\bar{\Gamma}\,\bar{M}\,\bar{K}$, as shown in Fig. 1(a). The calculation uses plane waves on a 2D surface with a hexagonal array of triangular potential barriers, whose strength is the only fitting parameter [7]. The model allows a straightforward computation of the change in the surface electron energy when the superlattice parameter is varied. We obtain an electron energy gain of 0.31 meV/atom when going from the 9×9 to the 9.5×9.5 structure, i.e., of the order of the energy needed to slightly compress the Ag overlayer in the latter [2].

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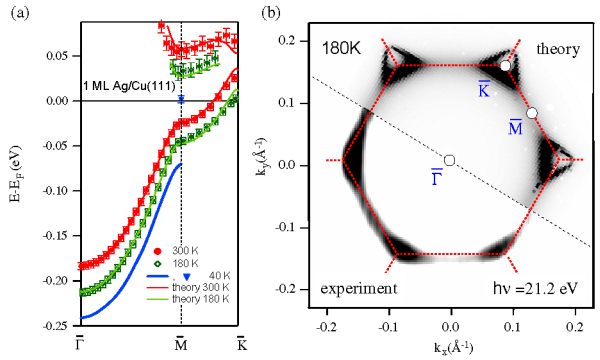

FIG. 1 (color online). (a) Band structure along $\bar{\Gamma}\,\bar{M}\,\bar{K}$ for 1 ML Ag/Cu(111) at various temperatures. The data at 40 K have been taken from Ref. [1]. The thin lines that fit data points at 180 and 300 K are deduced from a simple theoretical model [7]. (b) Photoemission intensity image at the Fermi energy taken at 180 K (lower-left half) compared to the theoretical Fermi surface (upper-right half).

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[1] A. Bendounan, F. Forster, F. Reinert, B. Kierren, Y. Fagot-Revurat, and D. Malterre, preceding Comment, Phys. Rev. Lett. **96**, 029701 (2006).
[2] F. Schiller *et al.*, Phys. Rev. Lett. **94**, 016103 (2005).
[3] A 50 meV shift at $\bar{M}$ with a 0.5° misorientation can be obtained only by assuming a free-electron band at $k_{\|} = 0.15$ Å^{-1}. But at $\bar{M}$, the surface bands are much flatter, with a total dispersion of only 30 meV along $\bar{M}\,\bar{K}$.
[4] R. Paniago *et al.*, Surf. Sci. **336**, 113 (1995).
[5] We performed a careful fit using two Lorentzian lines of the same width convoluted with the Fermi-Dirac distribution to the $\bar{M}$-point spectrum measured by A. Bendounan *et al.*, Phys. Rev. B **72**, 075407 (2005). We obtain $E_{\bar{M}} = 2 \pm 4$ meV, in disagreement with Ref. [1].
[6] C. R. Ast and H. Höchst, Phys. Rev. Lett. **90**, 016403 (2003).
[7] J. Cordón *et al.* (to be published).

