Comment on "Atomic-Structure-Dependent Schottky Barrier at Epitaxial Pb/Si(111) Interfaces"

Under ultrahigh vacuum Pb is known to grow on Si(111) according to the layer-plus-islands mode. The islands sit in parallel epitaxy with (111)Pb$\parallel$(111)Si: [$1\bar{1}0$]Pb$\parallel$[$1\bar{1}0$]Si. The two-dimensional (2D) adlayers, which are essentially close-packed Pb layers according to a recent surface x-ray-diffraction study,[1] display, at saturation, two structures: At room temperature (RT) a commensurate Pb/Si(111)7×7 structure, in parallel orientation relative to the substrate, is formed while it is after annealing or high-temperature (HT, $\sim$250°C) deposition an incommensurate Pb/Si(111)$R30°$-i one, rotated by 30°.

Above these two different adlayers, over *n*-type samples, Heslinga *et al.*[2] have deposited, *in situ*, Pb contacts and further determined from electrical measurements, current-voltage (*IV*) and capacitance-voltage (*CV*). The following Schottky-barrier heights were found: 0.62 $\pm$0.02 eV (*IV*), 0.70$\pm$0.02 eV (*CV*) on the first phase [they call these Si(111)7×7 Pb contacts] and 0.90 $\pm$0.02 (*IV*), 0.93$\pm$0.01 (*CV*) on the second one [they call these Si(111)$\sqrt{3}\times\sqrt{3}R30°$-Pb contacts]. They underline that 0.93 eV is an extraordinarily high Schottky-barrier and attribute the large difference, by at least 0.23 eV, in barrier heights between the two types of contact to the different interfacial geometries and related electronic structures.

At the time they submitted their Letter, Heslinga *et al.*[2] were probably not aware of our just published results[3] on synchrotron-radiation photoemission measurements of the formation of the Pb/Si(111) interface at RT and HT where similar Schottky-barrier heights (SBH's) were mentioned. At that time we had indicated from Si 2*p* core-level spectroscopy on *p*-type substrates a gradual shift towards lower binding energy of the Si 2*p* line upon completion of the Pb/Si(111)7×7 phase at RT. In further works[4,5] we have obtained the same result on *n*-type samples and noticed an additional band-bending shift (by $\sim$0.1 eV) after annealing or upon HT deposition in the course of the obtention of the Pb/Si(111)$R30°$-i phase.

As the Fermi level (FL) at clean Si(111)7×7 surfaces is pinned at 0.65 eV above the valence-band maximum[6] these band-bending changes lead straightforwardly to the following SBH's at saturation of the two 2D adlayers: $\sim$0.87 and $\sim$0.97 eV, respectively, to be compared to the values cited above obtained by Heslinga *et al.* on diodes.

If the tendency towards higher barriers after annealing is the same, large discrepancies exist between the values measured, especially at RT, by photoemission (0.87 eV) on the monolayer films and by electrical measurements on thick diodes (0.7 eV). These discrepancies surely point to drastic structural changes in the first layers below the islands during their growth—the metastable Pb/Si(111)7×7 initial phase surely disappears—a reorganization must occur also for the annealed Pb/Si(111)$R30°$-i phase to recover a parallel orientation of the islands [as a matter of fact such a rearrangement was envisaged for the related Pb/Ge(111) interface[7]]. As a consequence we think that the difference measured by Heslinga *et al.* on their two types of contacts cannot be simply assigned to the two different structures of the 2D adlayers.

With photoemission we can probe electronic states only in the monolayer regime; indeed our valence-band spectra[4] showed a marked difference in the occupied density of states for the two 2D phases, although both showed emission at the FL. These new metallic states pin the Fermi level at 0.25–0.15 eV above the valence-band maximum, yielding unusually large SBH's.

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[1]F. Grey, R. Feidenhans'l, M. Nielsen, and R. L. Johnson, J. Phys. (Paris) **50**, 7181 (1989).

[2]D. R. Heslinga, H. H. Weitering, D. P. van der Werf, T. M. Klapwijk, and T. Hibma, Phys. Rev. Lett. **64**, 1589 (1990).

[3]G. Le Lay, K. Hricovini, and J. E. Bonnet, Appl. Surf. Sci. **41/42**, 25 (1989).

[4]G. Le Lay, M. Abraham, K. Hricovini, and J. E. Bonnet, in Proceedings of the NATO Advanced Research Workshop on Kinetics and Growth at Surfaces, Acquafredda di Maratea, Italy, 1989, edited by M. Lagally, NATO Advanced Studies Institutes (to be published).

[5]K. Hricovini and G. Le Lay, in Proceedings of the Second European Conference on Progress in X-Rays Synchrotron Radiation Research, Rome, Italy, 1989 [Nuovo Cimento (to be published)].

[6]F. J. Himpsel, F. R. McFeely, J. F. Morar, A. Taleb-Ibrahimi, and J. A. Yarmoff, in "Photoemission and Adsorption Spectroscopy of Solids and Interfaces with Synchrotron Radiation," Proceedings of the International School of Physics "Enrico Fermi," Course CVIII, Varenna, Italy, 1988 (to be published).

[7]H. Huang, C. M. Wei, H. Li, B. P. Tonner, and S. Y. Tong, Phys. Rev. Lett. **62**, 559 (1989).