Local nature of artificial homojunction band discontinuities

M. Marsi
Department of Physics, University of Wisconsin, Madison, Wisconsin 53706

Gelsomina De Stasio
Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, 00044 Frascati, Roma, Italy

G. Margaritondo
Institut de Physique Appliquée, Ecole Polytechnique Fédérale, PH-Ecublens, CH-1015 Lausanne, Switzerland

(Received 27 December 1991; accepted for publication 29 April 1992)

The feasibility of creating homojunction band discontinuities by dipole intralayers was recently demonstrated with photoemission studies. We explored the nature of this intriguing mechanism by studying the effects of several complex intralayers, specifically stacked sequences of dipole intralayers. Quite unexpectedly, we found that the magnitude of the corresponding discontinuities is comparable to those created by individual dipole intralayers. We discuss this result in light of the recently observed [L. Sorba, G. Bratina, G. Ceccone, A. Antonini, J. F. Walker, M. Micovic, and A. Franciosi, Phys. Rev. B **43**, 2450 (1991)], similarly unpredicted saturation at low thickness of intralayer-induced heterojunction band discontinuities modifications.

I. INTRODUCTION

Recent successes in modifying and creating band discontinuities[1–7] have revolutionized the prospective for semiconductor band gap engineering.[8] The successes involved the controlled modification of heterojunction band discontinuities by ultrathin intralayers,[1,4,5] and the creation of artificial homojunction band discontinuities by dipolar double intralayers.[2,3,6,7] The interest of these results has stimulated experimental and theoretical[2,3,9] work to clarify the nature of the underlying phenomena. The experimental part of this work produced some unexpected results,[1] including those discussed in this article.

One method to explore the nature of the phenomena is to study their dependence on the intralayer thickness. In the case of heterojunction band discontinuity modifications, this approach was extensively used by Niles *et al.*;[5] more recently, Sorba *et al.*[1] found modifications that are much smaller than the theoretical prediction and tend to saturate for intralayer thicknesses approaching one monolayer. This confirms the local nature of the phenomena, as found by Niles *et al.*[5]

We extended the same approach to the case of the creation of homojunction band discontinuities. The present experiments consisted of measuring the band discontinuities induced by a double dipolar intralayer,[2,3,6,7] and then comparing the results to the corresponding ones produced by a sequential stack of two or three double intralayers, as illustrated in Fig. 1.

II. EXPERIMENTAL PROCEDURE AND RESULTS

The experimental approach, except for the use of sequences of double layers, is equivalent to that described in Refs. 6 and 7. The systems that we studied were Ga-P or Al-P dipolar double layers at Si-Si homojunctions.[7] A homojunction with a given double intralayer was prepared by taking a cleaved Si substrate, depositing the intralayer, and then a Si overlayer.

The creation and magnitude of the band discontinuities were deduced from core-level photoemission spectra of the two sides of the homojunction.[6,7] The core-level spectra, those from Si as well as those from the intralayer, also

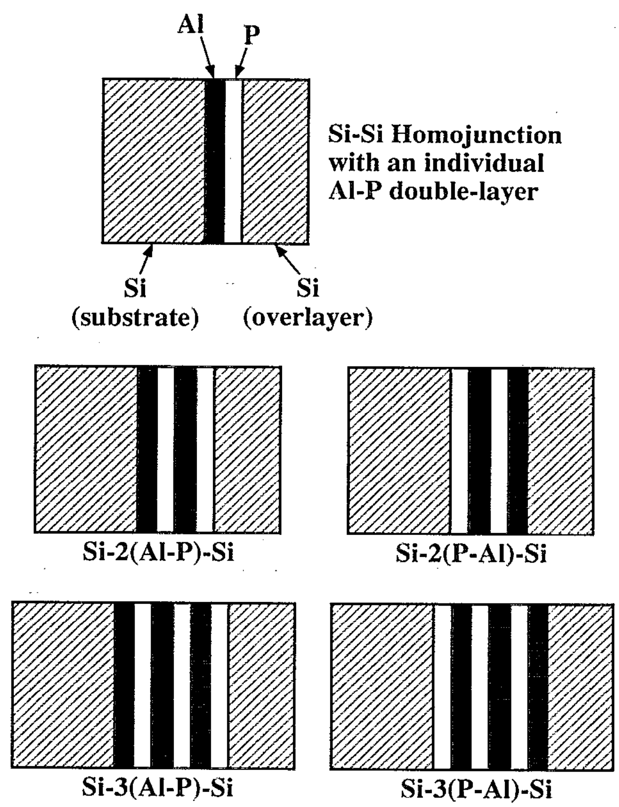

FIG. 1. Schemes of the structures investigated in the present experiments.

 0021-8979/92/161443-03$04.00

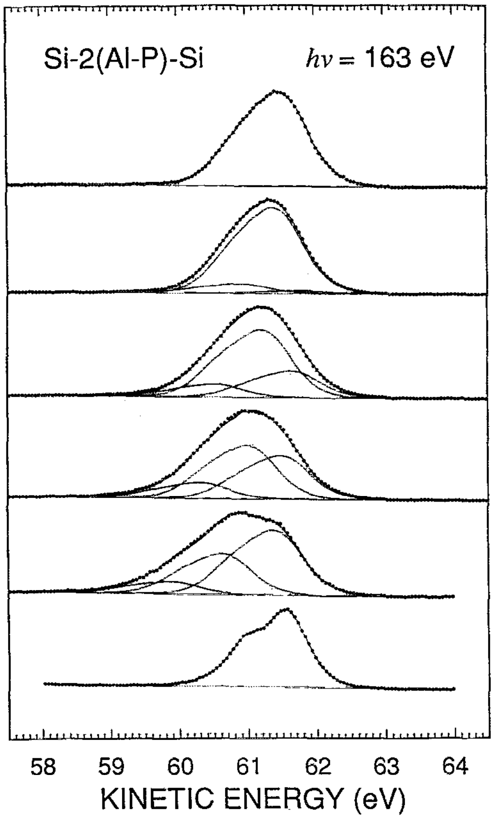

FIG. 2. Evolution of the Si 2*p* photoemission peak with increasing Si coverage after two stacked Al-P double layers have been deposited on cleaved Si(111). The photon energy was 163 eV. From bottom to top, the curves correspond to: cleaved Si with the two Al-P double layers; the same system with a thin Si overlayer of 1, 2, 3, and 5 monolayers; the same system with a thick Si overlayer.

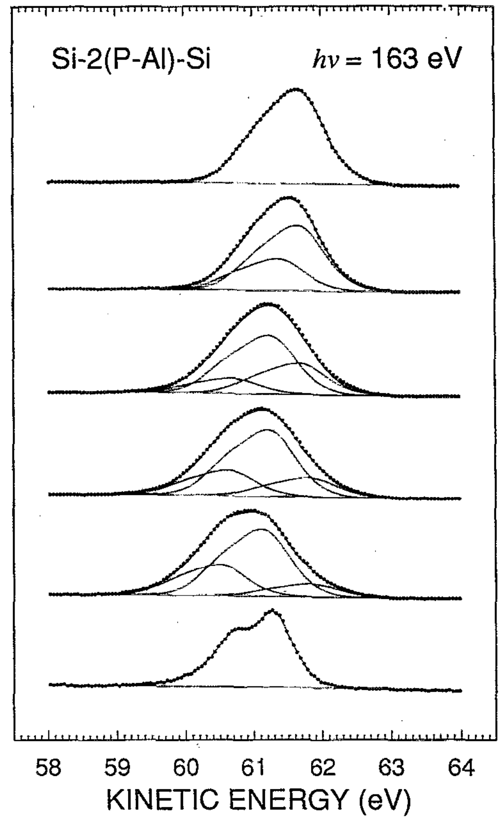

FIG. 3. Data corresponding to those of Fig. 2, but for the opposite intralayer deposition sequence: first P, then Al, P, Al. The sequence of Si overlayer thicknesses is 0, 2, 3, 4, 8 monolayers, followed by the thick overlayer spectrum.

provided information on the local chemistry and possible microdiffusion. All depositions were performed on room-temperature substrates, therefore they did not produce ordered (epitaxial) overlayers. As to the overall morphology of the interface, the intensity of the core-level photoemission peaks at different intralayer and overlayer thicknesses ruled out large amounts of interdiffusion.

Typical results are shown by Figs. 2 and 3 in the case of two stacked double layers, Al-P-Al-P and P-Al-P-Al [hereafter labeled as 2(Al-P) and 2(P-Al)]. The figures show Si 2*p* core level spectra, decomposed using a standard least-square fitting procedure as in Ref. 7. The results of the decomposition are in close correspondence to those found for individual double layers. In each case, we find three components: the one from the substrate that decreases in intensity with increasing overlayer thickness; then, a small component on the left-hand side due to a localized chemical species visible only for a limited range of overlayer thicknesses; finally, the component from the Si overlayer whose intensity increases with the overlayer thickness.

The energy separation between these two components corresponds to the misalignment of the band structures on the two sides of the homojunction. This fact has been repeatedly tested in previous studies of individual double layers.[6,7] For example, we verified that by inverting the deposition sequence of the intralayer's components, the misalignment was also inverted. We see the same result in Figs. 2 and 3. After inverting the deposition sequence, the small spectral component due to the interface chemical species is still on the extreme left-hand side, whereas the two other components are inverted, but the magnitude of their distance remains unchanged.

III. MAIN CONCLUSIONS

The most relevant result derived from Figs. 2 and 3 is the magnitude of the misalignment; that also corresponds to the magnitude of the artificial band discontinuities. We derive a value of 0.5 eV, and the value derived for the same systems in the case of an individual double layer was also 0.5 eV.[7] Experiments performed on 2(Ga-P) and 2(P-Ga) are fully consistent with those on 2(Al-P) and 2(P-Al); no substantial increase is observed on going from the individual double layers to two double layers.

We then repeated the test with three stacked double layers, and the results are shown in Figs. 4 and 5. The spectral components once again correspond to those of Figs. 2 and 3, and the derived discontinuity magnitude is the same, 0.5 eV. We then conclude that stacked double

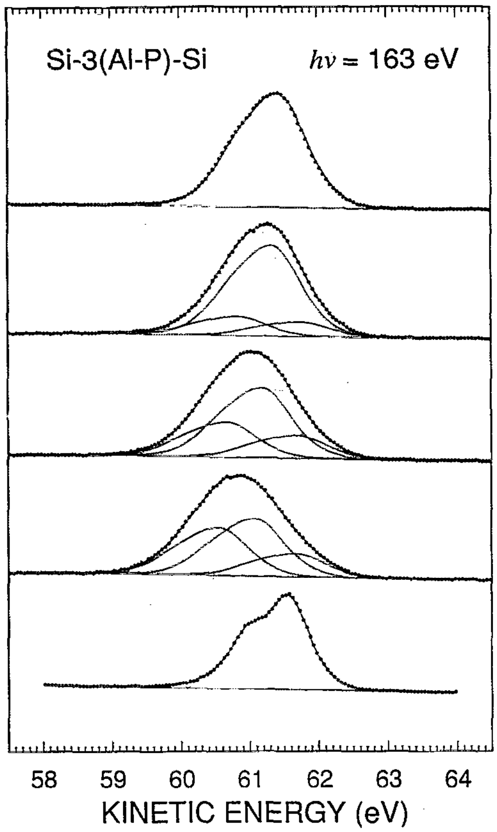

FIG. 4. Data corresponding to those of Fig. 2, but for three stacked Al-P double layers. Si overlayer thicknesses: 0, 2, 3, 5 monolayers, again followed by the thick overlayer spectrum.

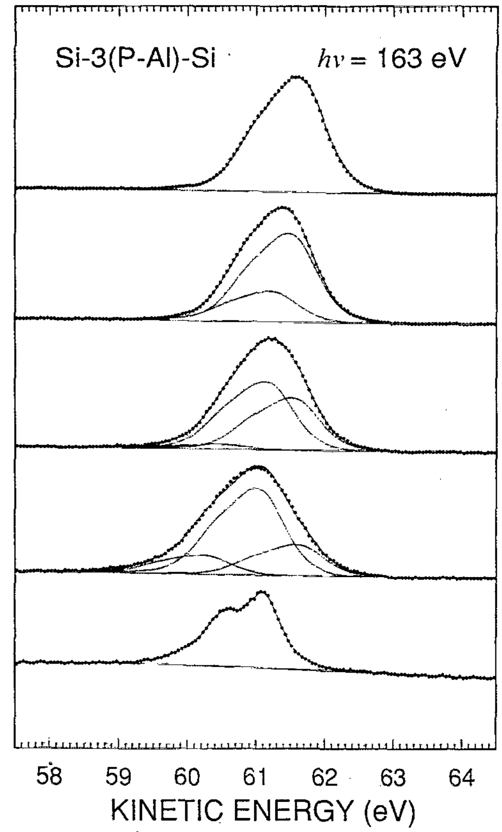

FIG. 5. The data for the intralayer deposition sequence opposite to Fig. 4: P-Al-P-Al-P-Al. Si overlayer thicknesses: 0, 2, 5, 8 monolayers plus the thick overlayer spectrum.

layers do not increase the effect of an individual layer, contrary to elementary predictions based on sequential dipoles.

This surprising result, on the other hand, is in agreement with a rather general trend: intralayer-induced modifications of heterojunction band discontinuities tend to saturate at 0.5–1 monolayer thickness.[1,4,5] This result disagrees with most of the theoretical models,[1] but one can propose some intuitive hypotheses for its explanation. One trivial point is that the effects must obviously saturate at some point because they cannot increase indefinitely; a reasonable magnitude of the saturation value is set by the distances between the band edges and the charge neutrality level,[10] which roughly corresponds to the saturation values of our artificial band discontinuities.

Somewhat correlated to this hypothesis is the fact that the dipoles are screened, and that the screening effects are not adequately described in terms of the dielectric function. We note that saturation effects are predicted for intralayer-induced band discontinuity intralayers by the theory of Muñoz and Rodriguéz-Hernández.[9] The origin of the similar effects found in the present work for artificial homojunction band discontinuities must be clarified by an *ad hoc* theoretical model that will probably contribute to our general understanding of local screening phenomena.

ACKNOWLEDGMENTS

This work was supported by the Fonds National Suisse de la Recherche Scientifique, by the National Science Foundation, by the Ecole Polytechnique Fédérale de Lausanne, and by the Italian National Research Council. The experiments were performed at the Synchrotron Radiation Center of the University of Wisconsin, a national facility supported by the National Science Foundation (NSF).

[1] L. Sorba, G. Bratina, G. Ceccone, A. Antonini, J. F. Walker, M. Micovic, and A. Franciosi, Phys. Rev. B **43**, 2450 (1991).
[2] S. Baroni, R. Resta, A. Baldereschi, and M. Peressi, in *Spectroscopy of Semiconductor Heterojunctions*, edited by G. Fasol, A. Fasolino, and P. Lugli (Plenum, New York, 1989), NATO Asi Series B, No. 206, p. 251.
[3] S. Baroni, R. Resta, and A. Baldereschi, *Proceedings of the Nineteenth International Conference on the Physics of Semiconductors*, edited by W. Zawadzki (Institute of Physics, Polish Academy of Sciences, Wroclaw, 1988), p. 525.
[4] P. Perfetti, C. Quaresima, C. Coluzza, C. Fortunato, and G. Margaritondo, Phys. Rev. Lett. **57**, 2065 (1986).
[5] D. W. Niles, M. Tang, J. McKinley, R. Zanoni, and G. Margaritondo, Phys. Rev. B **38**, 10949 (1988).
[6] J. T. McKinley, Y. Hwu, B. E. C. Koltenbah, G. Margaritondo, S. Baroni, and R. Resta, J. Vac. Sci. Technol. A **9**, 917 (1991).
[7] M. Marsi, S. La Rosa, Y. Hwu, F. Gozzo, C. Coluzza, A. Baldereschi, G. Margaritondo, J. T. McKinley, S. Baroni, and R. Resta (unpublished).
[8] F. Capasso and G. Margaritondo, *Heterojunction Band Discontinuities: Physics and Device Applications* (North-Holland, Amsterdam, 1987).
[9] A. Muñoz and P. Rodriguéz-Hernández (private communication).
[10] F. Gozzo, C. Coluzza, G. Margaritondo, and F. Flores, Solid State Commun. **81**, 553 (1992).