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Geometric structure of Be$(10\bar{1}0)$

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The structure of clean Be$(10\bar{1}0)$ was determined by low-energy electron-diffraction (LEED) $I(V)$ analysis and the result compared to first-principles calculations. Both theory and experiment indicate that from the two possible terminations of the truncated bulk, the one with the shorter first-interlayer spacing is realized. The values for the multilayer relaxations obtained by LEED essentially coincide with the theoretical prediction. Although the magnitude of the first- to second-layer relaxation fits well into the trend observed on other simple metal surfaces, the driving force is probably different for beryllium. [S0163-1829(96)02520-9]

Upon cleavage of a crystal, the atoms at the newly created surfaces tend to relax perpendicular from their bulk positions or even rearrange so that the lattice periodicity parallel to the surface changes. Developing an understanding of these so-called interlayer relaxations and reconstructions of clean surfaces is one of the most fundamental tasks in surface science. On most nonreconstructed surfaces, the distance between the first and second atomic layer, d_{12}, is observed to contract by a few percent, a general trend being that the more open the surface the larger this relaxation. However, on some surfaces an outward relaxation of the first layer has also been observed [e.g., Al(100) (Ref. 1), Al(111) (Refs. 2,3), Mg(0001) (Ref. 4) and Be(0001) (Ref. 5)]. Hannon and co-workers have shown that, for many metals, the change in the first-interlayer spacing is a linear function of the bulk interplanar spacing (both normalized to the nearest-neighbor distance).[5,6] In the present paper, we are not only concerned with the experimental observations, but also compare to state-of-the-art calculations. Therefore, Fig. 1 shows the ''universal curve'' for the simple metals together with the results of first-principles calculations.

Most of the qualitative explanations for the relaxations of clean surfaces predict a contraction of d_{12} (Refs. 7–9). The most widely accepted model was given by Finnis and Heine[8] and invokes a Smoluchowski-type charge smoothing mechanism[10] to account for the contraction of d_{12} on open surfaces: the electronic wave functions do not follow the corrugation of the first-layer atoms but, in order to lower their kinetic energy, smear out causing an electrostatic force, which drags the first-layer ions towards the bulk. Clearly, the importance of this effect should increase with surface corrugation, in qualitative agreement with the experimental findings.[5] As early as 1970, Lang and Kohn have shown that a small *expansion* of d_{12} may be found for metals with a high electron density, due to the outward pressure of the conduction electrons.[11,12] A combination of these models seems to

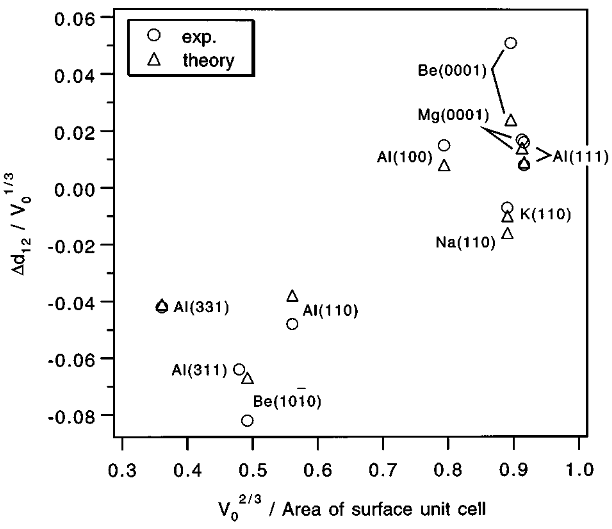

FIG. 1. A comparison of change in d_{12} as a function of the inverse area per unit cell, both normalized to the volume per bulk atom, V_0, for simple metals. The references for the points are Al(111) exp. (Ref. 2), th. (Ref. 43); Al(001) exp. (Ref. 1), th. (Ref. 43); Al(110) exp. (Ref. 44), th. (Ref. 43); Al(113) exp. (Ref. 45); Al(331) exp. (Ref. (46), th. (Ref. 47); Be(0001) exp. (Ref. 5), th. (Ref. 48); Be$(10\bar{1}0)$ this work; Na(110) th. (Ref. 49); K(110) exp. (Ref. 50), th. (Ref. 51); Mg(0001) exp. (Ref. 4), th. (Ref. 52).

give the trend for relaxations of all simple metal surfaces in Fig. 1: the points lie essentially on a straight line, with the exception of the two low electron-density alkali metals, where a smaller outward pressure of the conduction electrons leads to a decreased tendency for an expansion. However, neither of these concepts includes the effect of directional bonds, which should be important, at least for the transition metals,[13] and probably for beryllium.

Although beryllium is a simple metal with a high electron density, it is surprising that its surface relaxations follow the same trend as observed on Mg and Al, since its bulk properties are very different from those of a typical free-electron metal. The density of states shows a *minimum* at the Fermi level, the c/a ratio is the smallest among the hcp metals and the elastic properties indicate a substantial degree of covalent bonding. The main reasons for these anomalies are that Be has no p-core electrons and that the bonding between closed-shell beryllium atoms must be achieved by promoting $2s$ electrons into $2p$ states. The bonding energy, which compensates for this costly promotion, depends strongly on the coordination of the Be atoms. Hence, the physical properties of the Be surfaces may be expected to differ strongly from the bulk. Indeed, the (0001) surface has a *high* local density of states at the Fermi level caused by a free-electron-like surface state[14,15] and a large *outward* relaxation of the first layer is found.[5,16–19] Two different pictures as to the physical origin of this expansion have been given: Feibelman presented a bond-order bond-length consideration, keeping in mind that the bond length of a Be dimer is 11% longer than the nearest-neighbor distance in the bulk:[20] removing three-nearest neighbors of the surface atoms reduces the bonding energy, leads to a rehybridization, and increases the layer distance.[16] An alternative explanation is that, due to the surface states, the first layer is much more metallic than the bulk and will favor a more isotropic bonding. Consequently, the c/a ratio relaxes towards its ideal value. In this picture, the Be surface does not expand, it just returns to normal. An ideal c/a ratio at the surface would correspond to an expansion by 4%, slightly more than the calculated value.[18] The difference between this and the expansion of 5.8% determined by low-energy electron-diffraction (LEED) could be due to an additional outward pressure of the free electrons associated with the surface state around $\bar{\Gamma}$.

The $(10\bar{1}0)$ surface of beryllium has a higher corrugation than the (0001) surface. The first layer consists of closed-packed rows and the crystal may be thought of as a stack of such layers, very similar to an fcc(110) surface. The truncated bulk can be terminated in two ways, either with a short d_{12} (“short termination”) or with a long d_{12} (“long termination”) (Fig. 2). Just as on Be(0001), and independent of the termination, the local density of states has a maximum at the Fermi level, due to surface states[21] and we may except a significant contribution to the relaxation by these states. We have determined the type of termination and the multilayer relaxations of Be$(10\bar{1}0)$ by LEED $I(V)$ analysis and compared the result to first-principles calculations.

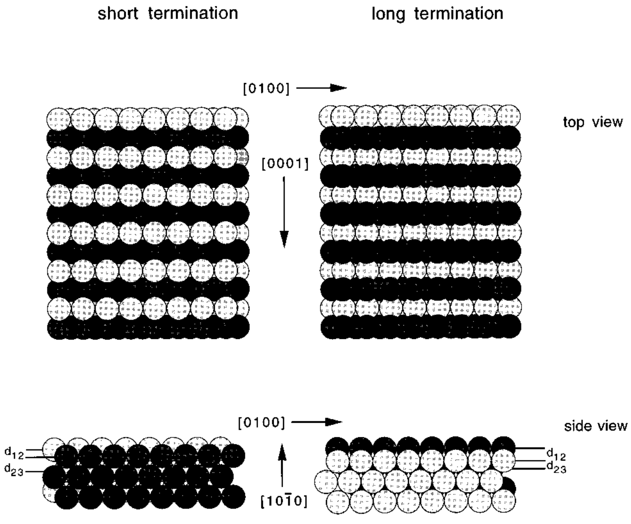

FIG. 2. Top and side view for the two possible terminations (“short” and “long”) of a hcp$(10\bar{1}0)$ surface. The shades correspond to the two different registries of the basal plane. The long termination may be constructed from the short termination by adding a layer of dark atoms. The side view is a cut along a basal plane.

The Be$(10\bar{1}0)$ sample was cut and polished by Geller MicroAnalytical Laboratories, Topsfield, MA. After removing the oxide layer by several hours of Ne$^+$-ion bombardment and annealing up to 950 K, the surface was cleaned by 20 min cycles of sputtering (0.5-keV Ne$^+$, 8 μa/cm^2) and annealing both at 760 K. This resulted in a sharp (1×1) LEED pattern and a clean surface judged by AES and EELS. Only a small amount of oxygen, estimated to be less than 4% of a monolayer, could not be removed. For the LEED measurements, the crystal was cooled to 120 K. The data were taken with a Video-LEED system developed at the University of Erlangen.[22] Before the actual measurements, the crystal was carefully aligned by an R-factor comparison between symmetry equivalent beams to ensure normal-incidence conditions. The final experimental data set was then formed by averaging over all accessible equivalent beams and consists of eight nonequivalent beams with a total-energy range of 1190 eV.

The LEED calculations were performed using the program package developed by Van Hove and Tong.[23,24] The atomic scattering phase shifts were provided by Müller and Heinz.[25] Two layers with a short spacing were treated as a composite layer and these were stacked by renormalized forward scattering.[23] For a first exploration of the parameter space, the same nonstructural parameters as in a recent investigation of the Be$(11\bar{2}0)$ surface structure[26] were used. Calculations for both terminations were performed over the whole physically reasonable range varying the first three-layer spacings on a grid of 0.03 Å. The structure giving the best reliability or R factor[27] for each termination was then refined on a grid of 0.01 Å. In case of the short termination, d_{45} was also allowed to vary from the bulk interlayer spacing in the final optimization. Since both the theoretical prediction (see below) and the experience from other hcp$(10\bar{1}0)$ surfaces[28–31] suggest a preference for the short termination, all nonstructural parameters were only optimized for this geometry. The atoms in the first two layers were assumed to have a different mean-square vibrational amplitude than the bulk atoms in the case of the short termination. For the long termination only, the atoms in the outermost layer had a mean-square vibration differing from the bulk. The bulk

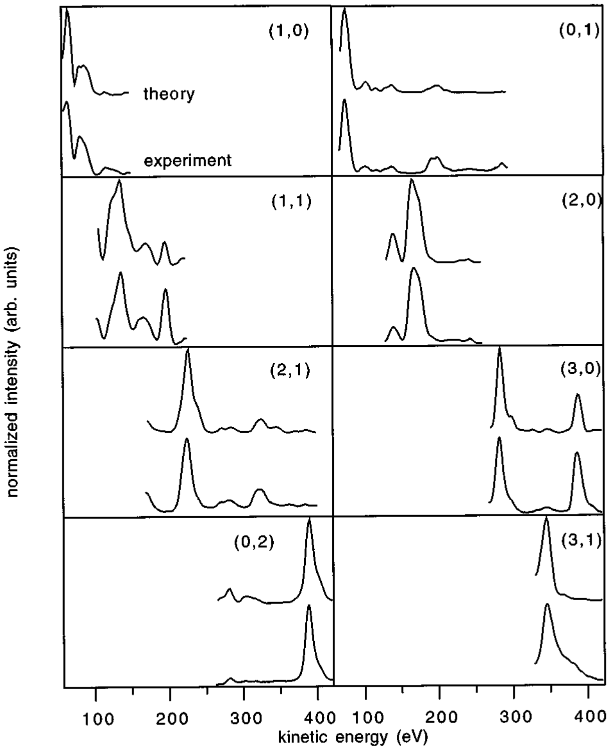

FIG. 3. Calculated (upper) and experimental (lower) $I(V)$ curves for eight nonsymmetry-equivalent beams. The intensity of each beam has been normalized individually. The calculation represents the result for the short termination with optimized relaxation parameters.

value was taken as 0.009 Å^2, corresponding to a Debye temperature of $\Theta_D = 1400$ K (Ref. 32). The imaginary part of the inner potential was taken to be $V_{\mathrm{Oi}} = 0.98$ eV $(E + V_{\mathrm{Or}})^{1/3}$, the real part is constant (10 eV) in the LEED program and was reoptimized as a linear function of the electron kinetic energy in the R-factor calculation routine. Finally, the structural parameters were again refined in order to assure convergence in all parameters.

The agreement between measured and calculated $I(V)$ curves was quantified by Pendry's R-factor R_P.[27] As a total R factor for all beams, the energy range weighted average of the individual R factors was taken. The measured $I(V)$ curves have been smoothed before applying the R-factor routine. The statistical errors in the structural parameters for the short termination were estimated by calculating the variance of R_P, $\mathrm{var}(R_P) = R_{P_{\mathrm{min}}}(8V_{\mathrm{Oi}}/\Delta E)^{1/2}$, and taking the interval where $R_P < R_{P_{\mathrm{min}}} + \mathrm{var}(R_P)$.[27] A possible correlation between the different parameters was not considered.

The result of the coarse exploration of the structural parameters shows a clear preference for the short termination: the lowest R factor is 0.28, for the long termination only a value of 0.54 could be reached. The refinement of the structure resulted in R factors of 0.26 and 0.52 for the short and long termination, respectively. The resulting $I(V)$ curves for the short termination together with the experimental data are given in Fig. 3. We find an oscillatory relaxation of the interlayer spacing; the precise values are given in Table I. The optimum value for the mean-square vibrational amplitude of the surface atoms is 0.017 Å^2 ($\Theta_D = 800$ K). Note, however, that the dependence of the R factor on this parameter is very small.

We tried to mix the optimized intensities of both termination in order to obtain information about a possible coexistence assuming, of course, that the size of the domains exceeds the transfer width of our LEED system. No improvement over the R factor of the short termination was found for the mixture and, judging by the R-factor variance criterion, less than 20% of the crystal area is terminated with a long interlayer spacing.

The first-principles calculations were based on density-functional theory within the local-density approximation (LDA) for the exchange and correlation potential.[33] The electron wave functions were expanded in plane waves with an energetic cutoff of 20 Ry. The Be atoms were described by soft separable pseudopotentials.[34–36] Generally, an orthorhombic supercell was used in the calculations with special **k** points[37] and the Fermi-surface smoothing technique of Methfessel and Paxton to integrate over the Brillouin zone.[38] A mesh of 6–24 **k** points was used in the irreducible quarter of the surface Brillouin zone. For the reconstructed surfaces, the number of **k** points was reduced to maintain identical sampling. The Kohn-Sham equations for the electronic wave functions were solved iteratively, applying a steepest-descent approach.[39–41] We used slabs of 18–22 layers (i.e., 9–11 double layers) thickness, separated by three double layers of vacuum. Six layers were relaxed on each side using a damped Newtonian dynamics technique.[41] This procedure gives a bulk lattice constant of $a = 2.238$ Å and $c/a = 1.573$. Hence, the ideal lattice spacings are 0.646 and 1.292 Å. For consistency, all calculated relaxations refer to these ideal theoretical values, rather than to the lattice parameters used in the LEED analysis. We have calculated the surface energies and relaxations for the short and the long termination. Since missing-row reconstructions are a common phenomenon on open surfaces, such as fcc(110) and Be$(11\bar{2}0)$, we have also calculated the surface energies for these structures even though they may be excluded by the (1×1) LEED pattern.

The first-principles calculations give essentially the same result as the LEED study. The short termination is clearly the more stable structure with a surface energy of 137 meV/Å^2, while the long termination gives a value of 235

TABLE I. Relaxations in percent for the short termination as a result of the LEED structure determination and the first-principles calculations. The error bars for the experimental values are given in parentheses.

	d_{12}	d_{23}	d_{34}	d_{45}
Experiment	-25 $(-4/+3)$	$+5$ $(-3/+5)$	-11 $(-5/+8)$	$+2$ $(-2/+4)$
Theory	-20	$+4.4$	-13	$+3.8$

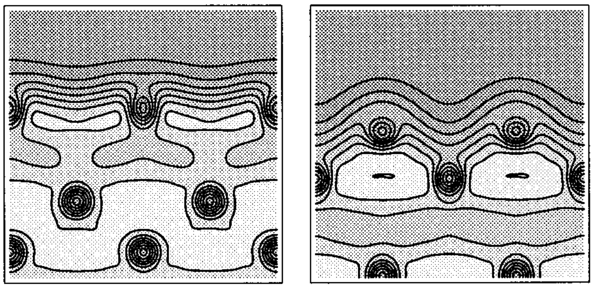

FIG. 4. Charge density contours for the short (left) and the long (right) termination of Be$(10\bar{1}0)$. The cut it is taken perpendicular to the close-packed rows. Note that first- and second-layer atoms are in a different plane, in case of the short termination (see Fig. 2). The difference between adjacent contour lines is 4×10^{-2} electrons/Å^3. The electronic charge is more corrugated for the long termination leading to a higher kinetic energy.

meV/Å^2. Both values refer to the relaxed geometry. The multilayer relaxations are also given in Table I. The relaxations contribute only a little to the surface energy. The energy gain, with respect to the truncated bulk configuration, is 31 and 20 meV/Å^2, for the short and long termination, respectively. The missing-row reconstructed surface is by about 15 meV/Å^2 less stable for the short termination. In case of the long termination, approximately 58 meV/Å^2 are gained. However, the reconstructed long termination is still less favorable than the unreconstructed short termination.

Both our LEED $I(V)$ analysis and the first-principles calculations show a clear preference for the short termination of the bulk Be crystal. The same termination is also found in all other structural studies of hcp$(10\bar{1}0)$ surfaces.[28–31] This may be a general rule, since two simple considerations favor the short termination: first, the kinetic energy of the free electrons at the surface should be lower, since the corrugation is a factor of two smaller (not taking into account relaxations) and the electronic wave functions are thus smoother. This is illustrated in Fig. 4 by a plot of the electronic charge density for both terminations. Second, by creating the long termination, the first-layer atoms lose six nearest neighbors, while they lose only 4 for the short termination. The second-layer atoms lose two nearest neighbors for both terminations. The lower coordination of the first-layer atoms leads to a higher energy for the long termination. The calculated energies for the missing-row reconstructed surfaces are consistent with this counting-of-cut-bonds approach: the long termination is instable to a reconstruction, because it reduces the number of cut bonds per surface area, whereas the unreconstructed short termination has less cut bonds than the reconstructed.

The agreement between LEED and the first-principles calculations as to the sign and magnitude of the relaxations is remarkably good. The numerical values of the relaxations seem to be very large at face value. However, we must not be mislead by the numbers: a 25% contraction of d_{12} is merely 25% of a rather small distance, i.e., 0.659 Å. Indeed, our result for Be$(10\bar{1}0)$ lies well within the range of the ''universal curve'' in Fig. 1. However, the fact that this beryllium surface shows quantitatively similar relaxations as free-electron metals, such as aluminum, is rather surprising since the driving force for the relaxation could be different: we have to keep in mind that we compare the *deviation* of d_{12} from the *bulk* interlayer spacing d_0. In aluminum, both the bulk and the surface have a high density of free-electron-like states at E_F, but in beryllium it is only high at the (0001) and $(10\bar{1}0)$ surfaces, whereas in the bulk the bonding is highly directional. Hence, the forces, which lead to the bulk interlayer spacing in beryllium, are very different from the forces dictating the distance d_{12}. According to Stumpf, the high electron density on Be(0001) leads to more isotropic bonding and the c/a ratio relaxes towards its ideal value. Here, the c axis lies parallel to the surface, such that a more isotropic bonding would mainly result into strain perpendicular to the closed-packed rows and it is difficult to speculate as to the effect on the relaxations perpendicular to the c axis. Both experiment and calculation indicate that the strain is not sufficiently high to induce a missing-row reconstruction.

Given the directional bonding in bulk beryllium, we might adopt a more ''chemical'' point of view. The simplest ''chemical'' concept is a bond-order bond-length consideration, as applied to Be(0001) by Feibelman. In the case of Be $(10\bar{1}0)$, it would predict an even larger expansion of d_{12} than on the closed-packed surface, because the number of nearest neighbors is even smaller. This is clearly not the case. However, we might try to pursue the ''chemical'' picture further and think of the bonding in beryllium in terms of partially filled sp and sp^2 hybrid orbitals, where the sp^2 orbitals are responsible for the bonding in the closed-packed layers, which are stacked perpendicular to the surface, and the sp orbitals achieve the bonding between these layers.[17,42] The creation of the surface then breaks bonds within and between the hexagonal layers and backbonding might lead to an inward relaxation of the first layer. However, in this picture, it is more suitable to describe the relaxations in terms of d_{13} and d_{35} referring to the changes of distances in the type of hexagonal layer containing the surface atoms and d_{24} for the other type of hexagonal layer and it is questionable if there is any hope to obtain a general picture of surface relaxations by comparing Δd_{12} for different crystal phases and surfaces as in Fig. 1.

In the present case, the first-principles calculations correctly predict both the termination and the magnitude of the relaxations correctly. On the closed-packed surface Be different calculations within LDA always give as smaller value of d_{12} than found by LEED.[16,18,17,19] Gradient corrections in the exchange-correlation potential lead only to a very small improvement,[17] but are also not expected to have a major effect on a close-packed surface. The reason for this discrepancy is not clear. A possibility would be that the LEED data have been taken at room temperature, while all the calculations were done at 0 K. A temperature-dependent analysis of the relaxation might give some indications as to the importance of temperature effects.[19] The clean Be$(11\bar{2}0)$ reconstructs,[26] so that it is not meaningful to compare the multilayer relaxations. However, it is interesting that the first-principles calculations (within LDA) fail to predict this reconstruction.[18]

In summary, we have determined the termination and multilayer relaxations of Be$(10\bar{1}0)$ by LEED and first-principles calculations. Both techniques show a clear preference for the short termination and give essentially the same relaxation parameters. Simple bond cutting and charge corrugation considerations indicate that the short termination might be a general rule for the hcp$(10\bar{1}0)$ surfaces. The change of the first-interlayer spacing, with respect to the bulk value, fits well into the trend observed on other simple metal surfaces, a fact which is rather surprising because, in the case of Be(0001) and Be$(10\bar{1}0)$, looking at Δd_{12} basically means comparing the properties of a free-electron-like metal in the first layers with a bulk material, which shows strong covalent bonding. A comprehensive picture of the multilayer relaxations of simple metal surfaces is still outstanding and it would be desirable to obtain more reliable data for the open surfaces of the alkali metals to study the effect of the electron density on the magnitude of the relaxations.

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