

Core-level study of MoSi₂ (001) and (110)

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Angle-resolved photoemission studies of the Si 2*p* and Mo 4*p* levels have been carried out on the (001) and (110) surfaces of a MoSi₂ single crystal using synchrotron radiation. Two surface-shifted Si 2*p* components were observed on both surfaces. The shifts were determined to be -0.26 and -0.68 eV for the (001) surface and -0.29 and -0.72 eV for the (110) surface. The reactivity upon oxygen exposure was investigated and the (110) surface was found to be most reactive. No shifted Mo 4*p* component could be detected either in the clean or in the oxidized spectra from any of these surfaces.

INTRODUCTION

The electronic and structural properties of refractory transition-metal silicides have received a great deal of interest^{1,2} during the last decade. Silicide formation at the interface between Si and transition metals is of great technological interest for the semiconductor industry.^{1,2} Therefore much work has been done to investigate transition-metal silicides.³⁻¹⁰ Mostly, surfaces of thin films reacted *in situ* or bulk polycrystalline samples have been investigated⁵⁻⁹ and only a few studies have been carried out on silicide single crystals.^{3,4} Some experimental and theoretical investigations of MoSi₂ (Refs. 5, 9, and 10) have been reported earlier. In order to further elucidate the surface electronic properties of MoSi₂, we have performed high-resolution core-level studies of two single-crystal surfaces.

Below we present the results of angle-resolved core-level-photoemission studies of the (001) and the (110) surfaces of a MoSi₂ single crystal. Clean surfaces were prepared *in situ* by sputtering and annealing cycles. For both surfaces two Si 2*p* components shifted towards lower binding energy were revealed. On the (001) surface, however, a weak third component shifted towards higher binding energy was also observed. The intensity ratios extracted for the Si 2*p* components at different photon energies indicate that the shifted components originate from the surface region. For the Mo 4*p* level no surface-shifted component could be detected. Upon oxygen exposures the (110) surface showed the highest reactivity and the Si 2*p* spectra recorded indicated Si oxidation on both surfaces. No oxide peak could be observed in the Mo 4*p* spectra even at the largest exposures investigated. These results are presented and discussed below.

EXPERIMENT

The experiments were performed at beamline 41 at the synchrotron radiation facility MAX-laboratory in Lund, Sweden. This beamline is equipped with a toroidal grating monochromator with three interchangeable gratings

giving photon energies ranging between 15 and 200 eV. The analyzer used is a hemispherical electron analyzer with an acceptance angle of $\pm 2^\circ$. The overall resolution is dependent of the operational parameters, but when recording Si 2*p* spectra it was selected to be ≤ 0.23 eV. When recording the Mo 4*p* or oxidized Si 2*p* spectra an overall resolution of, respectively, 1.0 and 0.55 eV was selected. The binding energies specified below are referenced to the Fermi level.

Single crystals of MoSi₂ were grown in a floating-zone growth mode in a He atmosphere with a pressure of 1 MPa. The preform for the floating-zone growth was made from a stoichiometric mixture of Mo 99.7% (Fluka) and Si 99.99% (Topsil), which was pressed isostatically to rods at 500 MPa and sintered in He at 1500 °C for 12 h.¹¹ The crystals were spark cut, mechanically polished, and checked with Laue to be within 1° of the (001) and (110) directions. The crystals were cleaned *in situ* by 10 min of sputtering followed by annealing at 1100 and 900 °C for the (001) and (110) surface, respectively. The temperature was measured with a pyrometer. This procedure resulted in clean and well-ordered surfaces as checked by photoemission and Low-energy electron diffraction (LEED). Both surfaces produced distinct 1×1 LEED patterns with low background intensities. Oxygen exposures were made at pressures ranging between 10^{-8} and 10^{-5} Torr, as read by the ionization gauge. The base pressure in the spectrometer was 2×10^{-10} Torr. The exposures are below given in Langmuirs (1 L = 10^{-6} Torr s). All measurements and exposures were made at room temperature.

RESULTS

Si 2*p* spectra recorded from the (001) and (110) surfaces at photon energies of 110 and 140 eV are shown by the dotted curves in Figs. 1 and 2, respectively. The shape of the more bulk sensitive 110-eV spectra indicates that at least three spin-split Si 2*p* components are contained in these spectra. This is also confirmed when using a curve-fitting procedure.¹² The experimental spectra

recorded from the (110) surface are found to be adequately modeled using three Si 2*p* components while for the spectra recorded from the (001) surface a weak fourth component is found to be needed when modeling the more surface-sensitive spectra. Of the spectra shown in Figs. 1 and 2, the 140-eV spectrum is the most surface sensitive.^{13,14} Using this, one can clearly distinguish the bulk component, labeled *B* in Figs. 1 and 2, and that the two low-binding-energy components, labeled *S1* and *S2*, are surface related. The weak component, labeled *S3* in Fig. 1(b), is only needed when fitting the most surface-sensitive spectra from the (001) surface and shows the largest surface-to-bulk intensity ratio at 140 eV. This component is further discussed below. A background consisting of the secondary-electron tail recorded using a photon energy of 114 eV has been subtracted from the 110-eV spectra shown in Figs. 1 and 2. An integrated background was applied in the curve-fitting procedure but is now shown in the figures.

For determining the surface shifts normal-emission spectra recorded at energies between 108 and 170 eV

were utilized. The fitting parameters used for all components were a spin-orbit split of 0.61 eV, a branching ratio of 0.5, a Lorentzian full width at half maximum (FWHM) of 0.07 eV, and an asymmetry parameter value of 0.03. Best fits to all these spectra were obtained when allowing a larger Gaussian width for the low-binding-energy component, labeled *S1*, while keeping the same Gaussian width for the other components. Gaussian FWHM's between 0.40 and 0.43 eV had to be used for the *S1* component while for the other components values between 0.28 and 0.38 eV were found to produce the best fits to the spectra recorded between 108 and 170 eV. Surface shifts for the *S2* and *S1* components of $-0.26(\pm 0.04)$ and $-0.68(\pm 0.05)$ eV were determined for the (001) surface and shifts of $-0.29(\pm 0.04)$ and $-0.72(\pm 0.06)$ eV for the (110) surface. The values given in the parentheses represent the maximum deviations obtained in the determinations. In an earlier study of the cleaved (001) surface only one surface-shifted component was observed, shifted -0.390 eV relative to the bulk component.¹⁵ This value is in between the values we have

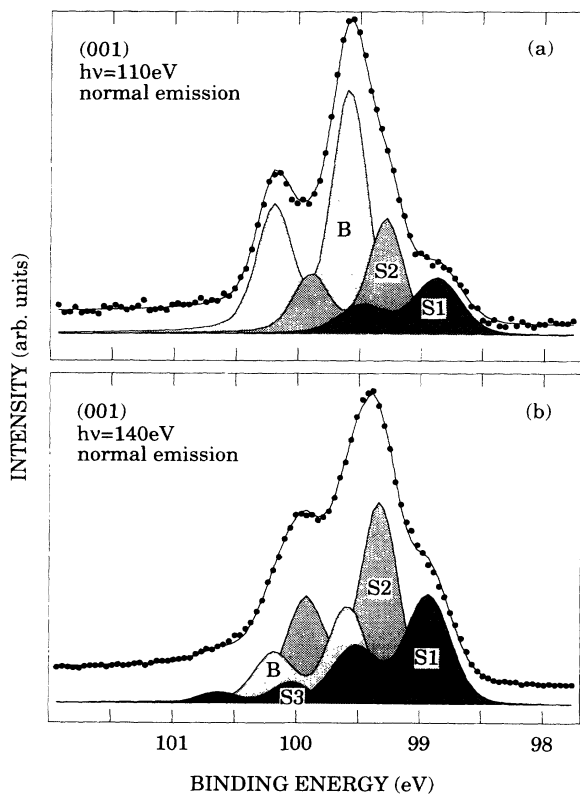


FIG. 1. Si 2*p* spectra recorded at normal emission from the (001) surface at a photon energy of (a) 110 eV and (b) 140 eV. The dotted curves show the data points, the solid curves through the data points represent the result of the curve-fitting procedure, and the shaded curves show the extracted bulk (*B*) and shifted (*S1*, *S2*, *S3*) components. Gaussian FWHM's of 0.29 eV for the 110-eV spectra and 0.31 eV for the 140-eV spectra are used, except for the component with the lowest binding energy, where a Gaussian of 0.40 is used for both spectra.

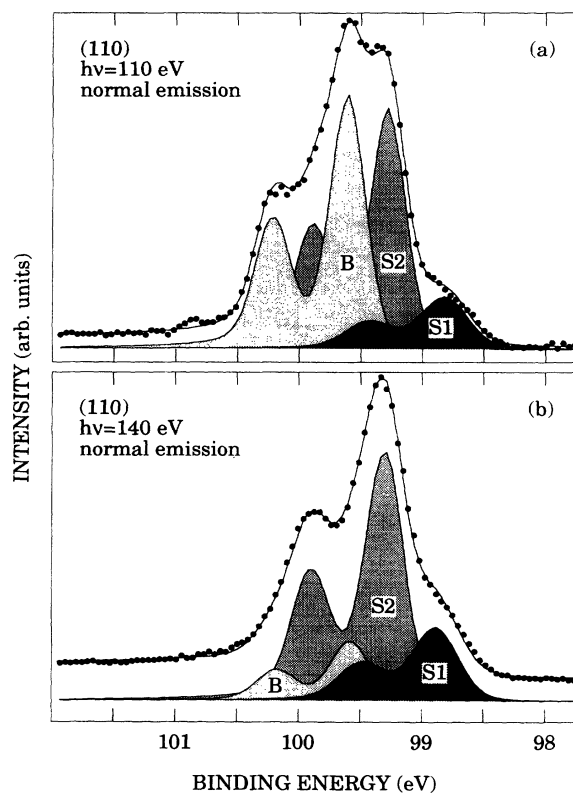


FIG. 2. Si 2*p* spectra recorded at normal emission from the (110) surface at a photon energy of (a) 110 and (b) 140 eV. The dotted curves show the data points, the solid curves through the data points represent the result of the curve-fitting procedure, and the shaded curves show the extracted bulk (*B*) and shifted (*S1*, *S2*) components. Gaussian FWHM's of 0.29 eV for the 110-eV spectra and 0.31 eV for the 140-eV spectra are used, except for the component with lowest binding energy, where a Gaussian of 0.40 is used for both spectra.

found in the present investigation of an annealed (001) surface. The binding energy of the bulk Si $2p_{3/2}$ level was determined to be $99.4(\pm 0.1)$ eV, which agrees well with the value of 99.36 eV determined in an earlier investigation.¹⁶

In order to investigate the reactivity of the surfaces, oxygen exposures were performed. Si $2p$ spectra recorded at a photon energy of 130 eV after different amounts of oxygen exposure are shown in Figs. 3(a) and 3(b). The spectra clearly show that the (110) surface has a higher oxidation rate than the (001) surface. On the (110) surface two pronounced silicon-oxide-related peaks are observed at approximately 1.9 and 3.4 eV higher binding energy than the Si $2p$ bulk peak at an oxygen exposure of 30 L. For the (001) surface 100 L of oxygen is needed before a silicon-oxide-related peak appears at about 3.0 eV higher binding energy than the Si $2p$ bulk peak. For the purpose of showing in more detail the effects of oxygen exposure on the (110) surface a difference spectrum has been constructed. This was made by first subtracting an integrated background from both the 30-L spectrum and

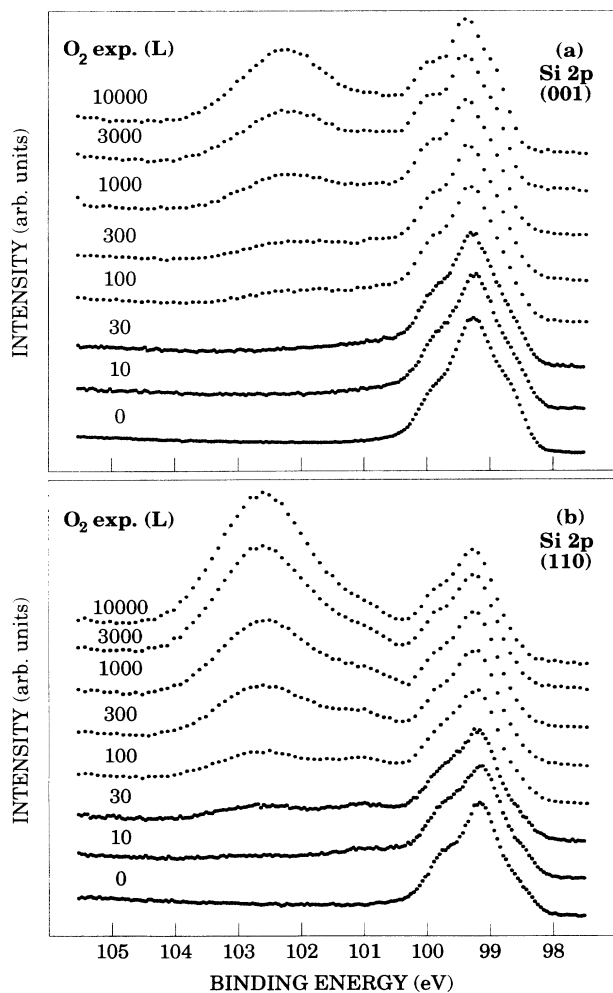


FIG. 3. Si $2p$ spectra recorded at normal emission after different oxygen exposures using a photon energy of 130 eV from (a) the (001) surface and (b) the (110) surface.

the clean spectrum and then normalizing the peak height before subtracting the clean spectrum from the 30-L spectrum. This difference spectrum is shown in Fig. 4, together with the results of a fitting procedure. To obtain a reasonable fit we had to add a third peak with a binding energy of 0.8 eV higher than the bulk peak. Thus three oxide-related peaks shifted +0.8, +1.9, and +3.4 eV relative to the bulk component are revealed. These results are in agreement with earlier work on Si surfaces¹⁷ where four oxidation states have been detected. These oxidation states showed Si $2p$ core-level shifts of 0.9, 1.9, 2.6, and 3.4 eV towards higher binding energy and were assigned to Si atoms bonded to 1, 2, 3, and 4 oxygen atoms.

Molybdenum spectra were recorded from both surfaces in order to investigate if surface-shifted levels could be detected and how these levels were affected upon oxygen exposure. Mo $4p$ spectra recorded at normal emission after different oxygen exposures using a photon energy of 95 eV are shown in Figs. 5(a) and 5(b). No surface-shifted level could be detected on either of the surfaces. The clean spectrum from the two surfaces appeared to be identical and this was confirmed by constructing a difference spectrum which resulted in a structureless line. No changes in the bulk component or appearance of an oxide-related peak could be revealed by constructing difference spectra between spectra recorded from the clean surface and after oxygen exposures. We therefore have to conclude that no surface-shifted or oxide-related molybdenum levels could be detected on these surfaces. When fitting the Mo $4p$ spectrum the parameters giving the best fits were a spin-orbit split of 2.0 eV, a branching

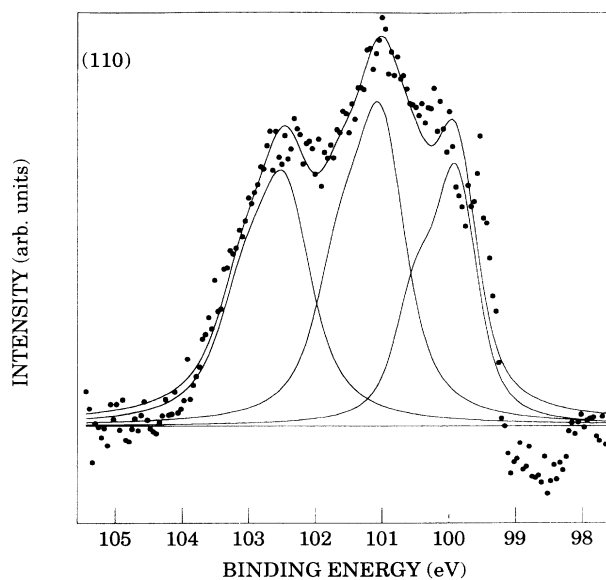


FIG. 4. Si $2p$ difference spectrum from the (110) surface between the 30-L spectra and a clean spectra using a photon energy of 130 eV is shown by the dotted curve. The solid line through the data points is the result of the curve-fitting procedure. The straight line is the zero and the three remaining curves show the oxide-related peaks.

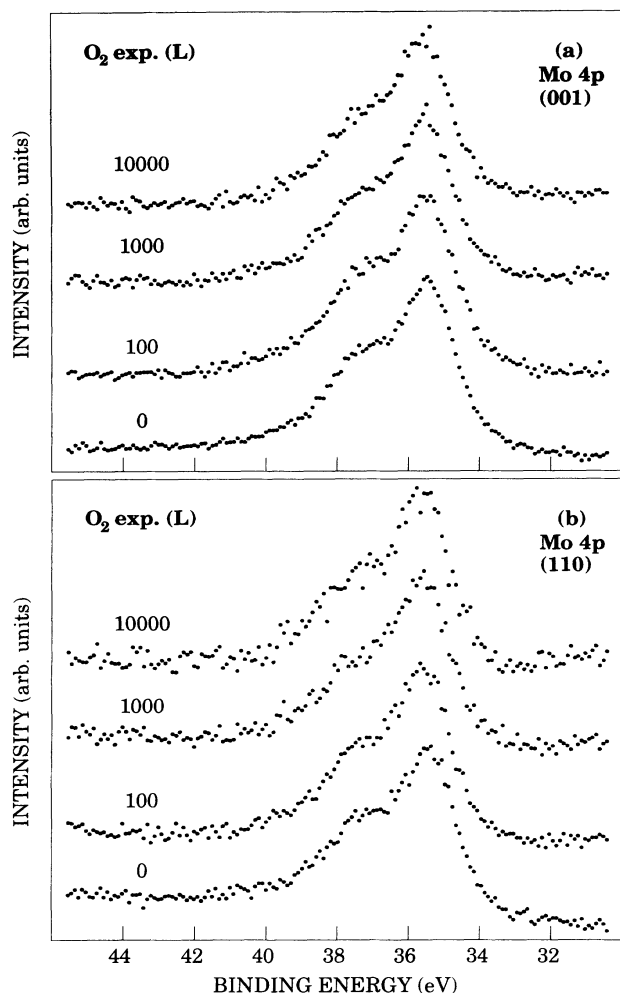


FIG. 5. Mo 4p spectra recorded at normal emission after different oxygen exposures using a photon energy of 95 eV from (a) the (001) surface and (b) the (110) surface.

ratio of 0.4, a Gaussian width of 0.9 eV, an asymmetry parameter of 0.07, and a Lorentzian width of 1.4 eV. These results differ slightly from earlier results obtained on Mo₃Si and MoSi₂ where a spin-orbit split of 2.1 eV and a branching ratio of 0.27 were reported.^{3,5} For the branching ratio our value is in closer agreement with the statistical value of $l/(l+1)=0.5$.

DISCUSSION

Two components shifted towards lower binding energy were observed in the Si 2p core level on both surfaces investigated. The intensity ratios extracted between the shifted and the bulk components at different photon energies clearly show that the shifted components are surface related. To be able to explain these shifted components we have to consider possible terminations of these surfaces. Si termination^{15,18} has been found in earlier investigations of MoSi₂, CoSi₂, and FeSi₂ surfaces cleaved *in situ* or cleaned *in situ* by ion bombardment and anneal-

ing. Our observations of surface-shifted Si 2p levels and initial oxidation of Si upon oxygen exposure, while no oxidation of Mo could be detected, also support this. Sharp 1×1 LEED patterns with low background intensity were observed from both surfaces. Below, we therefore assume perfect bulk termination, although the diffraction pattern observed does not exclude the possibility that overlayer structures compatible with the bulk diffraction pattern can exist.

Perfect bulk termination for the (001) surface would expose either a Mo or a Si layer. The stacking sequence consists of two Si layers followed by a Mo layer. This sequence is repeated but displaced one-half of the surface unit-cell diagonal. This builds the unit cell shown in Fig. 6. The Si atom sites in each layer are identical. This means that the atoms in one surface layer are expected to show the same core-level shift compared to the bulk peak. Assuming perfect bulk termination for the (110) surface exposes a mixed layer of Mo and Si; see Fig. 6. The Si atom sites in each layer are identical also in this case. This implies that if the surfaces were bulk terminated the experimentally observed shifts towards lower binding energies could be interpreted to originate from the two outermost layers. The component S1 would originate from the surface layer and S2 from the second layer. However, the intensity ratios extracted between S1/S2 would then indicate the amount of Si atoms to be less in the surface layer than in the second layer, which cannot be the case for bulk truncated surfaces. A Si overlayer structure, resulting in a not completely filled layer, could possibly explain these intensity ratios.

For the (001) surface a weak component, labeled S3, shifted towards higher binding energy by $0.44(\pm 0.05)$ eV, had to be added when fitting spectra recorded at photon energies ≥ 120 eV. Its relative intensity compared to the bulk component was ≤ 0.05 at 120 eV, showed a maximum of 0.22 at 140 eV and, thereafter, slowly decreased to 0.15 at 170 eV. The surface sensitivity is ex-

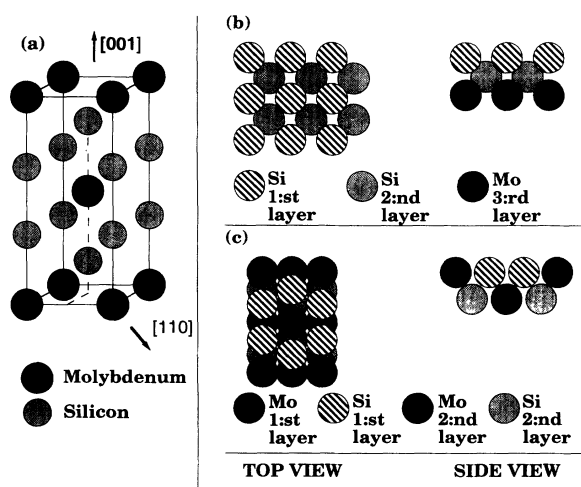


FIG. 6. (a) The crystal structure of MoSi₂, (b) top and side view of the (001) surface assuming the surface is terminated with two Si layers, (c) top and side view of the (110) surface.

pected to be maximal for spectra recorded at photon energies of about 140 eV (Refs. 13 and 14) and to decrease when going towards higher or lower photon energies. We can therefore conclude that also this component is surface related but its small relative intensity makes us discard the possibility that it originates from a complete surface layer. We cannot, however, discard the possibility that it originates from a surface layer almost depleted of Si atoms. This component shows a positive shift while the two other components showed negative shifts. A different origin can, therefore, be considered. Can different silicides be formed in the surface region during the cleaning procedure? It has been found earlier that Si tends to be enriched on the surface of sputtered annealed surfaces.^{15,18} In our case, the only stable silicide with more silicon in it than MoSi₂ is MoSi₃. Earlier investigations of chromium silicides^{4,7,19} indicate that the binding energy of Si 2*p* increases with an increasing amount of silicon. We would therefore expect to observe a component shifted towards higher binding energy if MoSi₃ was formed in the surface layers. This may explain the S3 component observed but since no value for the binding energy of Si 2*p* in MoSi₃ has been published we cannot conclude that this is the case. The two other components observed, S1 and S2, are shifted towards smaller binding energies and cannot be explained by MoSi₃ formation. No S3 component was observed on the (110) surface and a possible explanation can be that the (110) surface was annealed to 900°C while the (001) surface was annealed to 1100°C during the cleaning process.

To model surface shifts a thermochemical model has been proposed^{20,21} that expresses the surface shift as a sum of partial shifts. The dominating partial shift is often that originating from the loss of coordination at the surface^{20,21} and can be expressed as

$$\Delta E_v = c_v^* (E_{\text{coh}}^{z^*} - E_{\text{coh}}^z),$$

where c_v^* is a parameter that describes the loss of coordination at the surface compared to the bulk ($c_v^* = 1$ means total loss of coordination), E_{coh}^z is the cohesive energy of a z solid, and $E_{\text{coh}}^{z^*}$ is the cohesive energy of a z^* solid, where z^* denotes a z metal with a core electron removed and a valence electron added. Assuming perfect bulk termination for both surfaces and Si termination for the (001) surface yields c_v^* values of, respectively, 0.5 and 0.2 for the (001) and (110) surface, due to loss of 5 out of 10 and 2 out of 10 of the nearest neighbors. A cohesive energy per atom for MoSi₂ of 5.62 eV is obtained when adding the cohesive energy of two silicon atoms (9.26 eV) and one molybdenum atom (6.82 eV) (Ref. 22) and then subtracting the enthalpy of formation [$3 \times (-0.456 \text{ eV})$] (Ref. 23), and finally dividing this value by 3. In the same way a cohesive energy of 5.31 eV per atom is obtained for MoP₂. Using these values the model predict shifts of -0.16 and -0.06 eV for the (001) and the (110) surface, respectively. The model thus predicts a negative surface shift for both surfaces but a much smaller magnitude than the shifts determined experimentally. This behavior of the model, predicting the correct sign but a smaller magnitude than the experimental shift, has been observed

earlier.^{3,4} From the above we cannot draw any unambiguous conclusions about the origin of the shifted Si 2*p* components. A probable explanation for the S1 and S2 components is that they originate from the two topmost surface layers but other possibilities cannot be excluded.

The (110) surface was found to be more reactive than the (001) surface. We interpret this to be due to a larger amount of Mo atoms in the (110) surface layer. The Mo atoms are believed to dissociate the oxygen molecules into more reactive oxygen atoms which then bond to the Si surface atoms.²⁴ When assuming bulk termination the (001) surface is less closely packed than the (110) surface (Fig. 6) and could therefore have been expected to show a higher oxidation rate. The (001) surface has only one atom per surface unit cell while the (110) surface has six atoms per surface unit cell. The (110) surface cell is only 3.5 times larger than the (001) surface unit cell, which means that the (110) surface is more closely packed, by a factor of 1.7, than the (001) surface. Our results indicate, however, that the dissociation of oxygen in the vicinity of metal atoms is more important to the oxidation rate than the packing of the surface.

Since the same experimental parameters as used in this investigation of MoSi₂ have been used in earlier investigations on Cr₃Si and Mo₃Si (Refs. 3 and 4) it is worthwhile to compare the parameters obtained that produced best fits to the Si 2*p* spectra. The same Lorentzian broadening and spin-orbit split have been used in these fitting procedures. The asymmetry parameter of 0.03 used on MoSi₂ is much lower than the asymmetry parameters of 0.12 used for Cr₃Si and Mo₃Si.^{3,4} However, since the density of states at the Fermi edge is much lower for MoSi₂ than for Cr₃Si and Mo₃Si this seems reasonable since the asymmetry originates from electron energy losses at the Fermi energy. The Gaussian FWHM's needed to fit the Si 2*p* spectra in the earlier investigations^{3,4} were found to be smaller. At a photon energy of 130 eV, Gaussian widths of 0.31 (*B* and *S2*) and 0.40 eV (*S1*) were used for the different Si 2*p* components for MoSi₂ while values of about 0.24 eV were used in Refs. 3 and 4. The difference in width of especially the *S1* component, interpreted to originate from the surface layer, is so large that extra structures might well be hidden within this component. Of course, it cannot be ruled out that other effects might be the cause of this extra broadening, such as vibrational effects or a certain degree of disorder in the surface region. These latter effects may also explain why the width of the bulk and subsurface components is somewhat larger in MoSi₂ than in Cr₃Si and Mo₃Si.

SUMMARY AND CONCLUSION

Angle-resolved core-level-photoemission studies on the (001) and (110) surfaces of a MoSi₂ single crystal have been reported. Two surface-shifted components were detected for both surfaces. Surface shifts of -0.26 and -0.68 eV were determined for the (001) surface while shifts of -0.29 and -0.72 eV were obtained for the (110) surface. Negative surface shifts were predicted when using a thermochemical model but with much

smaller magnitudes than the experimental shifts. Si oxidation was observed upon oxygen exposures and a large difference in oxidation rate for the two surfaces was found. The (110) surface showed the highest oxidation rate. This was interpreted to be due to a larger amount of molybdenum atoms in the (110) surface, which act as catalysts to dissociate oxygen molecules to more reactive atomic oxygen. On the (110) surface three Si oxidation states could be identified. No surface-shifted or oxide-

related Mo 4*p* structure could be identified on either of the surfaces.

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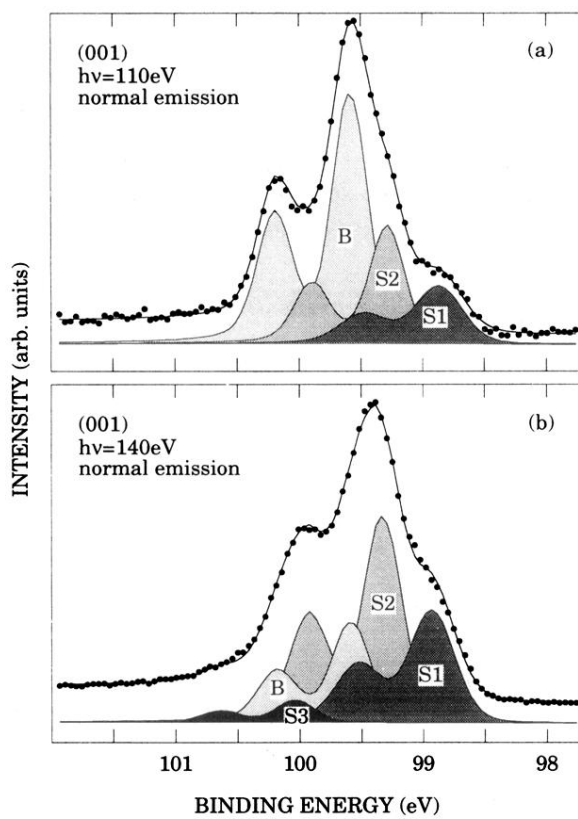


FIG. 1. Si $2p$ spectra recorded at normal emission from the (001) surface at a photon energy of (a) 110 eV and (b) 140 eV. The dotted curves show the data points, the solid curves through the data points represent the result of the curve-fitting procedure, and the shaded curves show the extracted bulk (B) and shifted ($S1, S2, S3$) components. Gaussian FWHM's of 0.29 eV for the 110-eV spectra and 0.31 eV for the 140-eV spectra are used, except for the component with the lowest binding energy, where a Gaussian of 0.40 is used for both spectra.

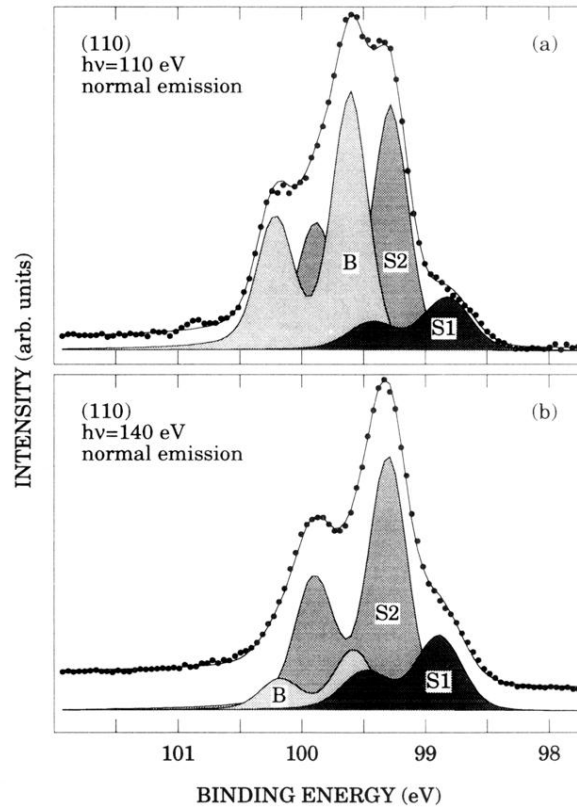


FIG. 2. Si $2p$ spectra recorded at normal emission from the (110) surface at a photon energy of (a) 110 and (b) 140 eV. The dotted curves show the data points, the solid curves through the data points represent the result of the curve-fitting procedure, and the shaded curves show the extracted bulk (B) and shifted ($S1, S2$) components. Gaussian FWHM's of 0.29 eV for the 110-eV spectra and 0.31 eV for the 140-eV spectra are used, except for the component with lowest binding energy, where a Gaussian of 0.40 is used for both spectra.

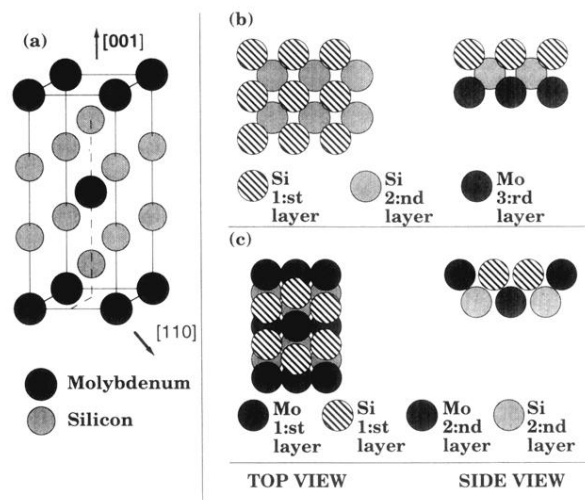


FIG. 6. (a) The crystal structure of MoSi_2 , (b) top and side view of the (001) surface assuming the surface is terminated with two Si layers, (c) top and side view of the (110) surface.