Sites, mobilities, and cluster formation of In atoms on a stepped Cu(100) surface

M. Breeman and D. O. Boerma
Nuclear Solid State Physics, Materials Science, Center, Nijenborgh U, 9747 AG Groningen, The Netherlands
(Received 8 January 1992)

The surface sites in In atoms deposited to a coverage of 0.013 monolayer onto a stepped Cu(100) surface were determined with low-energy ion scattering. This was done for various deposition temperatures in the range 63–300 K. The mobilities of In atoms on the terraces and along steps were deduced from the deposition-temperature dependence of the fractions of In atoms occupying different sites. It was found that, with increasing temperature, In adatoms first migrate to step edges to form one- and two-dimensional clusters and then are incorporated into the terraces at near-substitutional sites.

I. INTRODUCTION

For a better understanding of low-temperature epitaxial growth, and also of the kinetics of surface reactions, it is important to know the surface sites and the mobilities of deposited or adsorbed atoms. The trapping of such atoms at surface imperfections, and the formation and stability of small clusters of atoms, can be especially determinative for the structure and morphology of the overlayers formed during prolonged growth. From a simple calculation of random walk of surface atoms it can be estimated that, for a coverage of $<10^{-3}$ monolayers (ML), no clustering of deposited atoms will occur. At coverages of $\approx 10^{-2}$ ML, the early stages of cluster formation are expected to be visible. Only a few techniques are suitable for determining surface sites or structures at coverages of 10^{-2} ML or less. These include field-ion microscopy,[1,2] scanning tunneling microscopy,[3,4] and x-ray diffraction,[5,6] which have as a common feature that it is difficult to distinguish between different species of atoms at the surface. Recently, Schatz and collaborators reported perturbed-angular-correlation (PAC) measurements on radioactive In atoms deposited to very low coverage ($\approx 10^{-4}$ ML) onto (stepped) surfaces of Cu single crystals.[7–11] They proposed four well-defined types of In atoms on a stepped Cu(100) surface:[11] adatoms, adatoms at a step edge, substitutional step edge atoms, and substitutional terrace atoms. The occupation of these different positions was found to depend on the temperature during deposition and on the anneal treatment.

In the present work, we used low-energy ion scattering of 6-keV Ne^+ ions, combined with at time-of-flight measurement of the scattered particles (LEIS-TOF),[12] to determine the precise sites of In atoms deposited to a coverage of ~ 0.01 ML onto a stepped (100) surface of a Cu single crystal. This was done for 12 deposition temperatures in the range 63–300 K. In order to extract the desired information with such a low coverage of adsorbate atoms, we had to use a special geometry to be described later. From the temperature dependence of the fractions of In atoms in different sites, we deduced mobilities of In atoms on the terraces and along steps. Information about the formation of In clusters at and in step edges was obtained by comparing the experimentally obtained fractions with the results of Monte Carlo calculations of In atoms diffusing along step edges.

II. EXPERIMENT

A. Setup and sample preparation

The Cu single crystal was polished parallel to a (17,1,1) plane with an accuracy of better than 0.1°. The sample was baked and sputter cleaned in an UHV system (2×10^{-10} mbar), and finally mounted on a three-axes goniometer connected to a closed-cycle He refrigerator. With this cooling system, the sample can be cooled *in situ* to temperatures as low as 60 K. From low-energy-electron-diffraction patterns it was concluded that a surface was obtained, consisting of (100) terraces with an average length of 8.5 interatomic distances and monatomic steps, as is expected for a (17,1,1) surface. Indium atoms were evaporated with a calibrated Knudsen cell to a coverage of 0.013 ± 0.002 ML, at a substrate temperature of 63 K or higher. The In coverage was calibrated in the same UHV system by Rutherford backscattering. The temperature during evaporation and during the experiments was measured with a precision of ± 2 K with a Chromel-Au thermocouple in contact with the surface of the crystal.

B. Measurements and results

In the LEIS-TOF experiments, both neutral and ionized scattered Ne particles were observed at a backward angle of 155°. Azimuthal scans for Ne scattered from In were derived from spectra taken with a constant amount of beam charge, while rotating the crystal around the $\langle 100\rangle$ direction normal to the terraces. The polar detection angle α with the terraces was either 2° or 7° [see Fig. 1(a)]. The azimuthal angle φ with respect to the direction of the step edges was varied between $-24°$ and $+36°$ [indicated in Fig. 1(c)] with steps of 2°.

The Ne ions scattered from Cu and In atoms can be distinguished very well as separate peaks in the TOF spectra in the geometry specified above, even though the coverage of In atoms is only 1% of a ML. This is due to

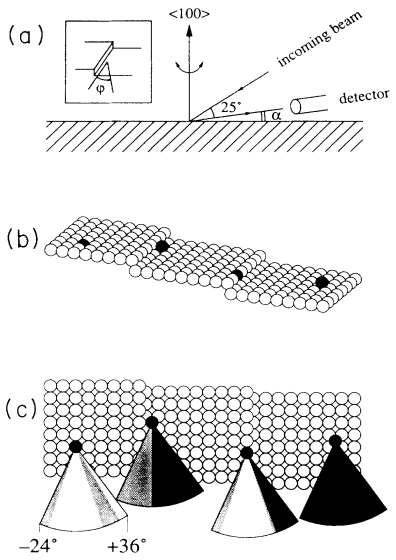

FIG. 1. (a) Geometry of the LEIS-TOF measurements. (b) Schematic view of a Cu(17,1,1) surface with In atoms (black) in four different positions. (c) Top view of the configuration of 1(b), with the expected angular distributions for In atoms in the different sites corresponding to (b) for the azimuthal range of $-24° < \varphi < 36°$. In the dark gray angular region, yield is expected for both polar angles α of 2° and 7°. In the light gray region, yield is expected for $\alpha = 7°$ but not for $\alpha = 2°$. In the white region, no yield is expected.

the fact that the Cu signal is largely suppressed by the use of the very glancing polar detection angles. Neon ions scattered from Cu atoms in the terraces are blocked on their way to the detector by neighboring surface atoms, and therefore the yield of in-terrace Cu atoms is zero. This is the case for both $\alpha = 2°$ and 7°. Neon particles scattered from atoms (Cu as well as In) which do not have neighbors in the direction of the detector can be detected. Therefore, atoms on this surface (adatoms) and atoms at or in step edges can be seen in a certain azimuthal range, as is indicated in Fig. 1(c). Atoms in different positions can be distinguished by their characteristic azimuthal angular distributions. As illustrated in Fig. 1(c), yield is expected for an In in-terrace atom for certain azimuthal angles at $\alpha = 7°$, while the yield of Cu in-terrace atoms is zero. This difference is due to the fact that In atoms are heavier than Cu atoms, and thus the energy of a Ne particle is higher after scattering from In than after scattering from Cu. This higher energy results in a narrower blocking cone, allowing the measurement of Ne scattered from In in case the azimuthal angle does not coincide with a close-packed string of surface atoms. Therefore, also the In in-terrace atoms can be positively identified by their azimuthal angular distribution for $\alpha = 7°$.

Summarizing, at the polar angles α used, the Cu signal is strongly suppressed by blocking by neighboring surface atoms, so the In signal can be well separated from the Cu signal. The four surface sites of In atoms, as proposed by Schatz and collaborators are shown in Fig. 1(b). The characteristic angular distributions expected for these sites, which enable us to distinguish between the different positions, are schematically shown in Fig. 1(c).

The azimuthal scans for Ne scattering from In were measured on a freshly prepared sample for 12 deposition temperatures T_D between 63 and 300 K. The measurements were performed at a temperature T_m of 63 K, or 100 K in case the deposition temperature was higher than 150 K. In order to prevent surface damage, the Ne dose per scan had to be restricted to 10^{13} ions/cm^2. For temperatures below 140 K, the ion-beam irradiation caused surface roughening. As described in more detail elsewhere,[13] Cu adatoms were observed to appear on the sur-

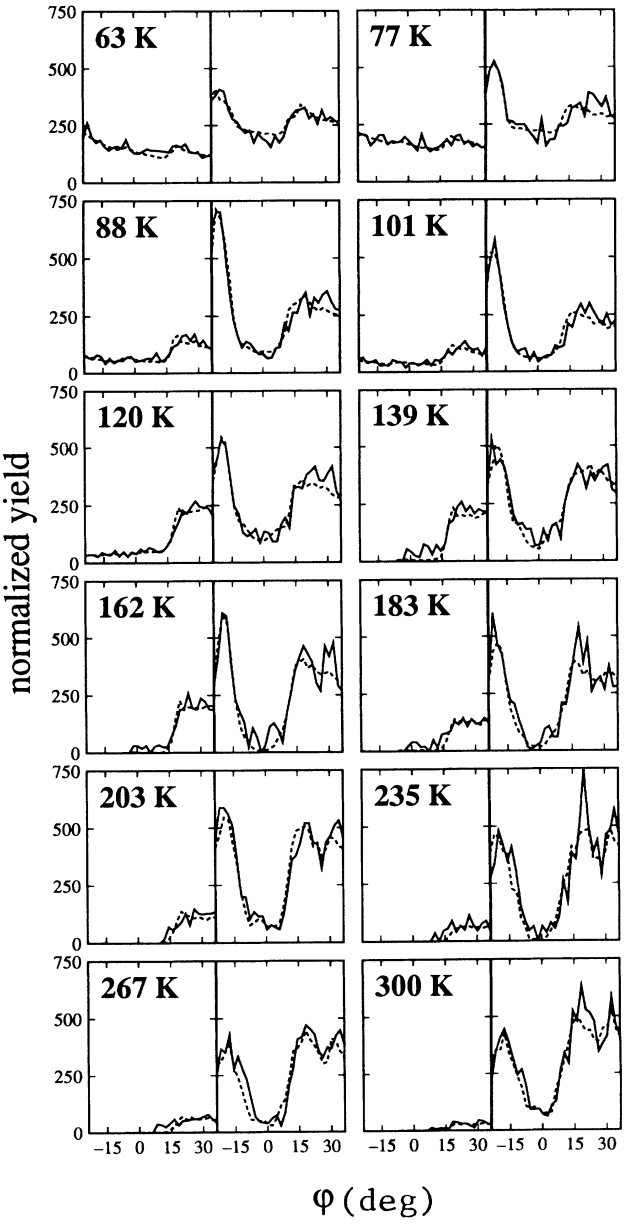

FIG. 2. Experimental scans (solid lines) and simulated scans (dashed lines) of 1.3% ML In on Cu(100) for different deposition temperatures. For each deposition temperature, the scans taken at a polar angle of 2° are displayed on the left-hand side; those taken at 7° are on the right-hand side.

face during ion-beam irradiation. These adatoms are interpreted to be self-interstitials, produced in the damage cascades, which have migrated to the surface. We determined an average number of 4.5 ± 1.5 Cu adatoms appearing on the surface per incoming Ne ion. From the temperature dependence of the Cu adatom coverage, we determined that Cu adatoms become mobile on a Cu(100) surface at $T=140\pm5$ K, form which we deduced an activation energy of 0.39 ± 0.06 for migration of Cu adatoms on a Cu(100) surface.

The azimuthal scans for the 12 deposition temperatures are displayed in Fig. 2. In the scans for $T_D \leq 120$ K and $\alpha=2°$, a yield due to adatoms, independent of φ, can be recognized. For $\varphi \geq 15°$, other scattering sequences, originating from In atoms at or in the steps, also contribute to the yield. These contributions are visible in all scans in the whole temperature region, for $\alpha=2°$. The big peak at $\varphi \approx -20°$ for $\alpha=7°$, visible for $T_D=63-183$ K, is caused by focusing by Cu step edge atoms, of Ne particles scattered from In atoms at or in the steps. The fraction of atoms in in-terrace positions, giving no yield for $\alpha=2°$, shows up in an almost pure form for $T_D>250$ K in the scans for $\alpha=7°$.

III. ANALYSIS

For assumed positions of In atoms with respect to neighboring Cu or In surface atoms, the azimuthal scans can be calculated rather precisely by means of Monte Carlo simulations.[14] In these calculations, binary collisions with all atoms within a distance of 2 Å, including those in second or deeper layers, are taken into account. The In atoms were assumed to occupy only positions on and in the topmost surface layer. The illumination with Ne ions of all atoms in this layer is assumed to be constant, because at incident angles of $\approx 30°$ shadowing of, and focusing effects on atoms in the first layer are insignificant. Since for backward scattering the impact parameter is small (<0.08 Å), we used the assumed position of the scattering (In) atom as the starting point of the calculation of the trajectories of the Ne particles to the detector. In this way, the trajectories are mainly determined by Cu-Ne interactions. The starting energy of the Ne particles was given by the energy of a 6-keV Ne atom after scattering over an angle of 155° by an In atom. The interatomic interactions were represented by the ZBL universal potential,[15,16] with the screening length for the Ne-Cu potential adjusted by a multiplication factor of 0.8. With this adjusted potential, measured azimuthal scans of Ne scattered from a clean Cu(100) surface were reproduced almost perfectly. For Ne-In interactions, we also took the ZBL universal potential with the screening length multiplied with a factor 0.8. In the simulations, the thermal vibrations of the Cu and In atoms were taken into account. The vibration amplitude of the Cu surface atoms was estimated by multiplying the bulk value with a factor of 2.07 for vibrations perpendicular to the surface, and a factor of 1.58 for in-plane vibrations, according to the model of Clark, Herman, and Wallis.[17] The value for the bulk vibrational amplitude for Cu was estimated using the Debye model with $\Theta_D=315$ K.[18] For atoms in the step edges, the component parallel to the steps was chosen to be the same as for in-plane motion of a surface atom. The other two components were given values as for vibration perpendicularly to the surface. The In vibration amplitudes were obtained by dividing the values for Cu atoms in corresponding positions with the square root of the mass ratio of In and Cu.

The azimuthal scans measured at polar angles $\alpha=2°$ and 7° were fitted simultaneously with scans calculated for the four In atom positions indicated in Fig. 1(b). In order to obtain good fits, it was found to be necessary to differentiate the in-step fraction into In atoms embedded in rows of In atoms, and rows of Cu atoms, respectively. Three configurations of rows of In atoms along steps were tried, and the only one which was found to fit our data consistently was a row of In atoms buckled perpendicularly to the surface. With this addition, an excellent fit to all measured scans was obtained, after fine adjustment of the In-atom positions. Also, other configurations have been tried in the fits, like a two-dimensional cluster of In atoms, and in-terrace In atoms adjacent to a vacancy. The quality of the fits was not improved significantly by these configurations, since the calculated scans were not sufficiently different from those for isolated In atoms in terraces.

The measured and fitted scans are compared in Fig. 2. The In-atom positions found are listed in Table I. The errors in these positions were derived from the variation with these positions of the normalized χ^2 values of the fits. As can be seen in Table I, all In-atom positions found are slightly elevated from the surface as compared with (extrapolated) Cu-lattice positions. This may be explained by the larger radius of In atoms as compared with Cu atoms (1.67 and 1.28 Å, respectively[19]), from which we expect shifts in the order of 0.3 Å or higher, depending on the degree of relaxation of the surrounding Cu lattice.

Since the experimental scans were normalized with respect to beam dose, and equal coverages of In atoms were used in all experiments, the contributions of the different components found in the fits should add up to the same, constant value for all deposition temperatures. This was found to be indeed the case within the limits of error, determined mainly by the uncertainty of about 10% in the In coverage. This is an additional reason to trust the results of the fits. It is also an indication that no In atoms are embedded in deeper layers.

From the fitting procedure, we have derived the frac-

TABLE I. Shifts of In atoms from (extrapolated) substitutional Cu positions.

Indium position	Upwards (Å)	Away from step (Å)
Isolated at step	0.40 ± 0.05	<0.05
Buckled row (low)	0.4 ± 0.2	0.10 ± 0.05
Buckled row (high)	0.8 ± 0.2	0.10 ± 0.05
Isolated in step	0.40 ± 0.05	<0.05
In terrace	0.45 ± 0.05	0

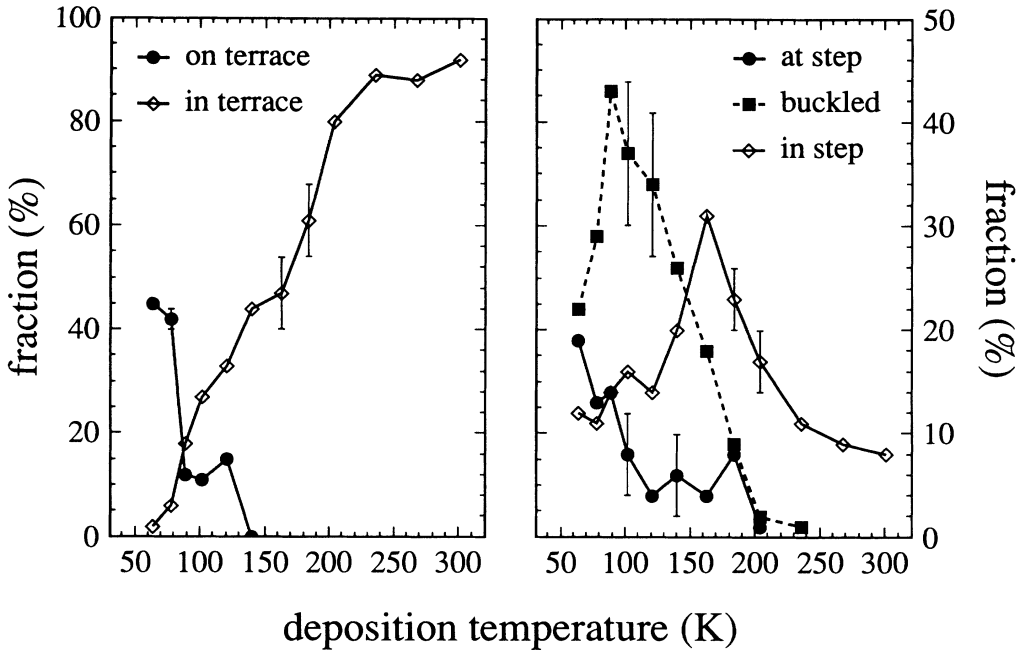

FIG. 3. Fractions of In atoms in different sites on a stepped Cu(100) surface.

tions of In atoms in the five sites as a function of T_D. These fractions are shown in Fig. 3. For $T_D \leq 77$ K, a large fraction of the In atoms is in adatom positions. For $T_D > 200$ K, almost all In atoms are incorporated in the terraces, with a small fraction of the In atoms in in-step positions. At intermediate temperatures (88–180 K), most In atoms were found to occupy at- and in-step positions, with a large fraction of the In atoms present in (buckled) rows of In atoms. This temperature dependence of the fractions reflects the migration of In adatoms, via clusters of In atoms at the step edges, to positions in the terraces.

From the temperature dependence of the In-adatom fraction, we have determined the activation energy for migration of In adatoms on a Cu(100) surface. From the fact that for temperatures $T_D \leq 77$ K a large fraction of In adatoms is observed, while at $T_D = 88$ K this fraction has decreased strongly, we conclude that In atoms become mobile on a Cu(100) surface at a temperature between 77 and 88 K. From the average number of jumps required for an adatom to reach a step edge, and the time the sample was kept at the deposition temperature (25 jumps and 600 s, respectively), the energy E for migration of In adatoms on a Cu(100) surface can be estimated. With an assumed attempt frequency of 10^{13} Hz, and an Arrhenius type of diffusion, we calculate this energy E to be 0.24 ± 0.03 eV.

Since the fraction of adatoms found for $T_D = 63$ and 77 K is $> 40\%$, it is concluded that at these temperatures In adatoms are immobile on Cu(100) terraces. However, the sum of the at-step and in-step fractions exceeds 50% at these temperatures, whereas a total of only 12.5% is expected for a stochastical distribution of deposited atoms. A possible explanation for this discrepancy is that In atoms arriving at the surface make jumps before they have lost their condensation energy of a few eV. It can be estimated that an average of about ten jumps is required to reproduce the observed adatom fraction. If jumps made after deposition take place in one direction only, as suggested by Egelhoff and Jacob,[20] then only a few jumps are required.

Another remarkable observation is the large fraction ($> 20\%$) of In atoms present in rows of In atoms after deposition at 63 or 77 K. This clustering requires mobility of In atoms along step edges at these low temperatures. Therefore, the activation energy for jumps along step edges must be lower than for jumps of adatoms over the (100) terraces. The lower activation energy for migration along steps may be understood in terms of the coordination number of the migrating atom. If the diffusion of an In adatom occurs via the hopping mechanism, which is very likely as will be argued below, the coordination number is reduced from 4 to 2 in the transition state. For migration along a step edge, the coordination number reduces only from 5 to 4 during the motion. Therefore, the latter process probably has a lower activation energy.

Recently, there have been many discussions about the atomic exchange mechanism for surface diffusion on fcc (100) surfaces.[21–23] From our data, we conclude that such an exchange mechanism, if present, is not the relevant process for the diffusion of In adatoms on a Cu(100) surface. Since almost all In atoms occupy near-substitutional terrace sites for $T_D > 200$ K, this site must be energetically favored for T_D below room temperature. If the diffusion of In adatoms would occur via the exchange mechanism, a substitutional Cu atom would change places with an In adatom, and vice versa. The latter step would be impossible at low temperatures, so

that the observed diffusion to the step edges cannot be explained with this mechanism.

The equilibrium site of In on a Cu(100) surface has been the subject of a recent paper by Li *et al.*[24] The authors calculate the binding energies of In atoms occupying various sites on a Cu(100) surface. The bridge site (fourfold hollow position) and the substitutional terrace site are found to compete energetically for In trapping, with the bridge site being the favored site. However, this is in contradiction with our observation that, for $T_D > 200$ K, almost all In atoms occupy near-substitutional terrace sites. Therefore, the equilibrium site of In on a Cu(100) surface must be the (near) substitutional terrace site, as proposed by Klas *et al.*[7]

IV. CLUSTERING OF IN ATOMS

For a further interpretation of the data, it should be kept in mind that In atoms in two-dimensional clusters at the step edges contribute in various ways to the fractions as observed with LEIS. This is illustrated in Fig. 4(a), in which two-dimensional clusters of In atoms at a step edge with kinks are depicted. For instance, In atoms within a cluster cannot be distinguished from in-terrace atoms, and atoms at the edges of a cluster in the direction of the detector will be seen as adatoms. The experimentally determined fractions represent the thermal equilibrium distributions for the deposition temperature T_D, frozen in at the lower measuring temperature T_m. During cooling, the fractions may change slightly, for instance by growth of clusters which are more stable at lower temperatures. We tried to reproduce the observed fractions by a Monte Carlo calculation of random walks of In atoms along step edges, or along In cluster edges, taking into account the "visibility" of In atoms in the various positions [see Fig. 4(a)], and the cooling down stage. In the calculations, the Cu atoms were assumed to be immobile. From the fact that Cu adatoms are only mobile for $T \geq 140$ K,[13] the assumption of Cu immobility seems reasonable for deposition temperatures below 130 K. We did not try to calculate the fractions for deposition temperatures higher than 130 K with our simple model, since for these temperatures mobility of Cu atoms in step edges and/or in terraces may come into play. In the calculations, the In atoms make periodic trial jumps to neighboring positions. The probability to arrive at a new position depends on the In-atom site and on temperature. The calculations for a temperature T_D were performed starting with a random distribution along step edges, until equilibrium was reached. They were then continued for a lower temperature T_m, with different probabilities for migration and sticking, until a new equilibrium was obtained.

The measured fractions were reproduced within the limits of error for all deposition temperatures $T_D < 130$ K under the following conditions: For $T_D = 63-77$ K, the In atoms at kink sites formed by Cu or In atoms are immobile, whereas single In atoms, and pairs of In atoms at steps, move with equal probability. Small (< 10 atoms) two-dimensional clusters are then formed at kink sites by In atoms which migrate along protruding step edges towards rows of In atoms which were already formed at the kinks [for a typical cluster, see Fig. 4(b)]. For the higher temperatures $T_D = 80-130$ K, the In atoms at kink sites can jump away from the kink or jump "kink upwards" with different temperature-dependent probabilities. With this additional degree of freedom, larger (up to ~ 20 atoms) two-dimensional clusters were found in the simulations. The different possible mobilities for In atoms in various positions are schematically shown in Figs. 4(b) and 4(c).

The results were found to be insensitive to variation in the assumed density of kinks in the steps between 0.5% and 5%. The deposition temperatures under consideration are well below the roughening transition temperature for a Cu(17,1,1) surface, which is in the order of 190 K according to the theory of Villain, Grempel, and Lapujoulade.[25] Therefore, we expect the kink density of the steps to be very low ($< 1\%$). However, since we did not cool our sample infinitesimally slowly from room temperature to the deposition temperatures, a few kinks in the

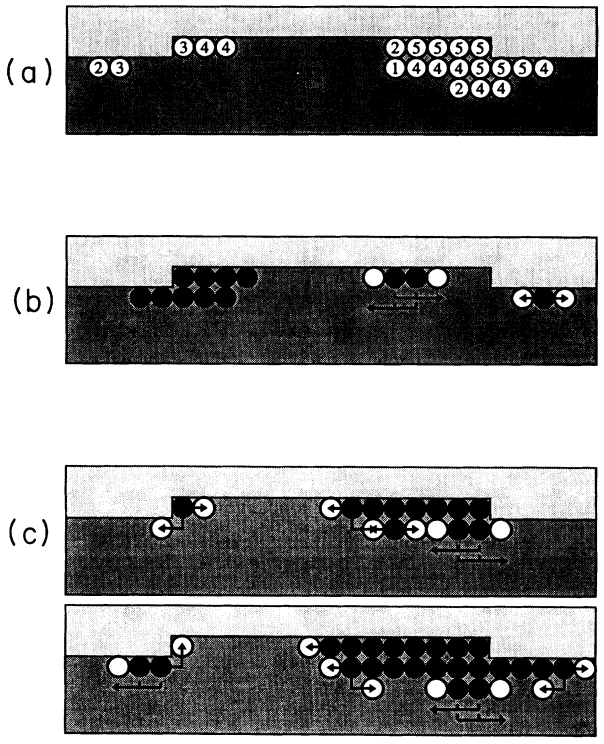

FIG. 4. Topview of a step edge with two kinks. The light gray part represents the upper terrace, and the dark gray part is the lower terrace. (a) Clusters of In atoms at step edges. The atoms are numbered, corresponding to the components to which they are expected to contribute if the detector is to the left. 1=adatom, 2=(isolated) at step, 3=in step, 4=buckled row, and 5=in terrace. (b) Mobilities of In atoms (black) as used in the Monte Carlo simulations for $T_D < 80$ K. The directions are indicated with arrows, and the destinations are shown as white circles. The pair of In atoms can move as a whole to a neighboring position. A typical cluster which is formed in the temperature region below 80 K is shown at the left kink. (c) Additional mobilities of In atoms as used in the Monte Carlo simulations for $T_D > 80$ K, including detrapping of In atoms from kink sites (formed by Cu atoms or In atoms).

step edges might be frozen in. From these considerations we estimate the kink density of the step edges to be between 0.5% and 5%.

V. COMPARISON WITH PAC RESULTS

Recently, Fink *et al.*[11] obtained similar data for a coverage of $\sim 10^{-4}$ ML of In atoms from perturbed-angular-correlation (PAC) measurements performed at temperatures between 77 and 300 K. Their results can be summarized as follows.

(a) An adatom fraction was observed at the same temperatures as in the present work. They deduced an activation energy for In-adatom migration on a Cu(100) surface of 0.28 eV, which is in good agreement with our value of 0.24 ± 0.03 eV.

(b) A fraction, interpreted as isolated atoms at steps or at kinks, was observed for temperatures in the range 77–200 K. According to our model, these atoms should be at kink positions. For temperatures above 100 K, this fraction is hardly present in our measurements, which is probably due to clustering.

(c) A fraction of In atoms in the steps was observed for temperatures between 120 and 270 K, which is in good agreement with our work.

(d) A fraction of In atoms in the terraces was observed only for temperatures of 180 K and higher, while we already see an in-terrace component at 100 K. This discrepancy can be explained by two-dimensional clustering of In atoms at the step edges. As stated before, in our measurements, In atoms in two-dimensional clusters cannot be distinguished from in-terrace atoms.

Summarizing, the results of the PAC experiments of Schatz and collaborators, and the LEIS results presented here, are in good agreement. The differences, especially in the behavior of the "at-step" and the "in-terrace" fractions, can be explained by one- and two-dimensional clustering of In atoms at the step edges, as was shown above by the Monte Carlo diffusion simulations. This clustering effect does not occur to a measurable extent for the 10^{-4}-ML coverage, which was used in the PAC experiments, as is revealed by Monte Carlo simulations of the diffusion process.

VI. CONCLUSIONS

In conclusion, we have shown that it is possible with LEIS to determine the surface sites of adsorbate atoms deposited to a coverage of only ~ 0.01 ML on a stepped substrate surface. This has been done for the case of In on a Cu(17,1,1) surface. The positions of the In atoms (see Table I) were found to be slightly shifted with respect to (extrapolated) Cu lattice positions. This can be explained by the larger radius of In atoms as compared with Cu atoms. It was found to be necessary to differentiate In atoms in step edges into In atoms embedded in rows of In, and rows of Cu, respectively. The only configuration of a row of In atoms along the steps which fitted our data consistently was a row of In atoms, buckled perpendicularly to the surface.

The mobilities of In atoms on the terraces and along steps were deduced from the temperature dependence of the observed fractions of In atoms in different sites. It was found that with increasing temperature, In adatoms first migrate to step edges to form one- and two-dimensional clusters, and then are incorporated in the terraces at near-substitutional sites. The activation energy for In-adatom migration on a Cu(100) surface was determined to be 0.24 ± 0.03 eV, which is in good agreement with the value of 0.28 eV deduced from PAC experiments in Konstanz. The diffusion of In adatoms on a Cu(100) surface is governed by the hopping mechanism, and not by the exchange mechanism. This is concluded from the presence of large at- and in-step fractions at temperatures at which mainly in-terrace atoms would be expected if the exchange mechanism would be the relevant process. It seems that even at deposition temperatures as low as 63 K, In atoms make a number of jumps before they have lost their condensation energy. From the fact that we observe clustering of In atoms at step edges at temperatures at which In adatoms are not yet mobile, and since such clustering requires mobility of In atoms along step edges, we conclude that the activation energy for migration of In atoms along step edges is lower than for In-adatom migration.

The measured fractions have been reproduced by means of Monte Carlo calculations of random walks of In atoms along step edges or along In cluster edges. The experimental fractions could be reproduced, assuming mobility of single In atoms and pairs of In atoms along steps for temperatures above 60 K, and detrapping of In from kink sites at temperatures above 80 K.

Finally, the present results are in good agreement with the results of PAC measurements of Schatz and collaborators. The differences (especially in the at-step and in-terrace fractions) can be explained by (one- and two-dimensional) clustering of In atoms at and in the step edges in the LEIS experiments. This clustering is not present in the PAC experiments, since the In coverage used was much lower.

ACKNOWLEDGMENTS

It is a pleasure to thank our colleagues at the University of Konstanz, in particular G. Schatz and R. Fink, for giving permission to quote their preliminary data prior to publication. The technical assistance of J. A. Reinders and L. Venema is highly appreciated. This work is part of the research program of the "Stitching voor Fundamenteel Onderzoek der Materie" (FOM) with financial support from the "Nederlandse Organisatie voor Wetenschappelijk Onderzoek" (NWO).

[1]R. Gomer, in *Proceedings of a NATO Advanced Study Institute on Surface Mobilities on Solid Materials, 1983,* edited by Vu Thien Binh (Plenum, New York, 1983), p. 127, and references therein.

[2]T. T. Tsong, Rep. Prog. Phys. **51**, 759 (1988), and references therein.

[3]D. D. Chambliss, R. J. Wilson, and S. Chiang, J. Vac. Sci. Technol. B **9**, 933 (1991).

[4]D. D. Chambliss and R. J. Wilson, J. Vac. Sci. Technol. B **9**, 928 (1991).

[5]S. Brennan, P. H. Fuoss, and P. E. Eisenberger, Phys. Rev. B **33**, 3678 (1986).

[6]W. C. Marra, P. H. Fuoss, and P. E. Eisenberger, Phys. Rev. Lett. **49**, 1169 (1982).

[7]T. Klas, J. Voigt, W. Keppner, R. Wesche, and G. Schatz, Phys. Rev. Lett. **57**, 1068 (1986).

[8]G. Schatz, T. Klas, R. Platzer, J. Voigt, and R. Wesche, Hyp. Int. **34**, 555 (1987).

[9]T. Klas, R. Fink, G. Krausch, R. Platzer, J. Voigt, R. Wesche, and G. Schatz, Europhys. Lett. **7**, 151 (1988).

[10]G. Schatz, in *Nuclear Physics Applications on Materials Science,* edited by E. Recknagel and J. C. Soares (Kluwer, Dordrecht, 1988), p. 297.

[11]R. Fink, K. Jacobs, G. Krausch, J. Lohmüller, B. Luckscheiter, A. Mayer, R. Platzer, B.-U. Runge, U. Wöhrmann, and G. Schatz (unpublished).

[12]D. O. Boerma, Nucl. Instrum. Methods B **50**, 77 (1990).

[13]M. Breeman and D. O. Boerma, Surf. Sci. (to be published).

[14]G. Dorenbos, M. Breeman, and D. O. Boerma, Nucl. Instrum. Methods B **64**, 88 (1992).

[15]J. F. Ziegler, J. P. Biersack, and U. Littmark, *The Stopping and Range of Ions in Solids* (Pergamon, New York, 1985), Vol. I.

[16]D. J. O'Connor and J. P. Biersack, Nucl. Instrum. Methods B **15**, 14 (1986).

[17]B. C. Clark, R. Herman, and R. F. Wallis, Phys. Rev. **139**, A860 (1965).

[18]J. W. Mayer and E. Rimini, *Ion Beam Handbook for Material Analysis* (Academic, New York, 1977).

[19]A. F. Wells, *Structural Inorganic Chemistry,* 5th ed. (Oxford University Press, Oxford, 1984).

[20]W. F. Egelhoff, Jr. and I. Jacob, Phys. Rev. Lett. **62**, 921 (1989).

[21]C. Chen and T. T. Tsong, Phys. Rev. Lett. **64**, 3147 (1990).

[22]G. L. Kellogg and P. J. Feibelman, Phys. Rev. Lett. **64**, 3143 (1990).

[23]P. Feibelman, Phys. Rev. Lett. **65**, 729 (1990).

[24]Yi Li, M. R. Press, S. N. Khanna, P. Jena, and M. Yussouff, Phys. Rev. B **41**, 4930 (1990).

[25]J. Villain, D. R. Grempel, and J. Lapujoulade, J. Phys. F **15**, 809 (1985).

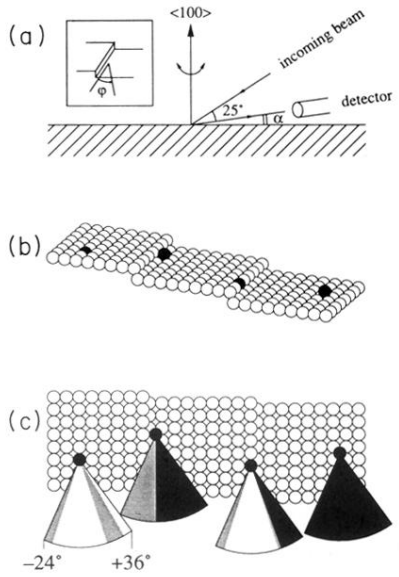

FIG. 1. (a) Geometry of the LEIS-TOF measurements. (b) Schematic view of a Cu(17,1,1) surface with In atoms (black) in four different positions. (c) Top view of the configuration of 1(b), with the expected angular distributions for In atoms in the different sites corresponding to (b) for the azimuthal range of $-24° < \varphi < 36°$. In the dark gray angular region, yield is expected for both polar angles α of 2° and 7°. In the light gray region, yield is expected for $\alpha = 7°$ but not for $\alpha = 2°$. In the white region, no yield is expected.

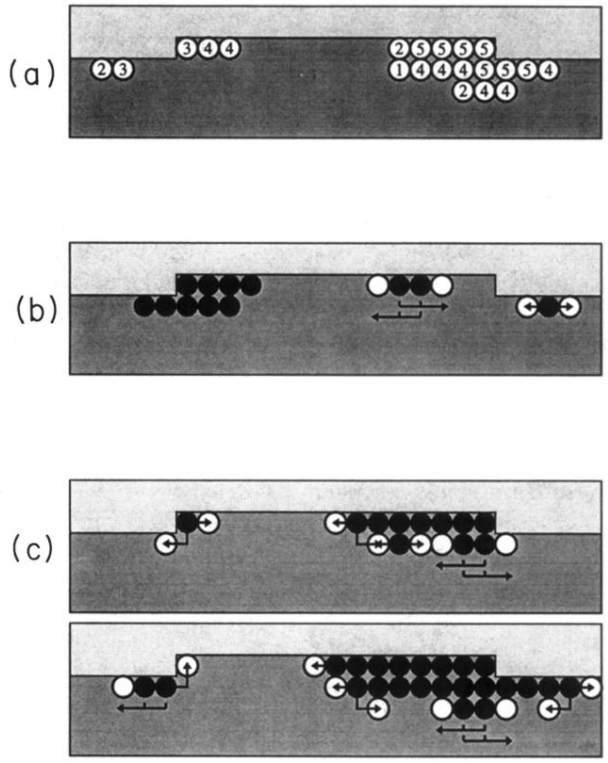

FIG. 4. Topview of a step edge with two kinks. The light gray part represents the upper terrace, and the dark gray part is the lower terrace. (a) Clusters of In atoms at step edges. The atoms are numbered, corresponding to the components to which they are expected to contribute if the detector is to the left. 1=adatom, 2=(isolated) at step, 3=in step, 4=buckled row, and 5=in terrace. (b) Mobilities of In atoms (black) as used in the Monte Carlo simulations for $T_D < 80$ K. The directions are indicated with arrows, and the destinations are shown as white circles. The pair of In atoms can move as a whole to a neighboring position. A typical cluster which is formed in the temperature region below 80 K is shown at the left kink. (c) Additional mobilities of In atoms as used in the Monte Carlo simulations for $T_D > 80$ K, including detrapping of In atoms from kink sites (formed by Cu atoms or In atoms).