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Adsorption and desorption of Se on $Si(100)2 \times 1$: surface restoration

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Abstract

This work entails a study of the adsorption of elemental Se on the reconstructed Si(100)2×1 surface. The investigation took place in an ultra high vacuum (UHV) by low energy electron diffraction (LEED), Auger electron spectroscopy (AES), thermal desorption spectroscopy (TDS) and work function (WF) measurements. The adsorption of one monolayer (1 ML) of Se at room temperature (RT) causes the transition of the reconstructed Si(100)2×1 surface to its original bulk terminated Si(100)1×1 configuration, while Se adatoms form a 1×1 structure by breaking the Si–Si dimer bonds. The Si–Se bond is strong (E_b =2.97 eV/atom), resulting in the formation of a SiSe compound. Above 1 ML, Se forms a SiSe₂ compound with E_b =2.67 eV/atom. The heating that follows causes the desorption of Se up until 1000 K, where Θ_{Se} =0.5 ML, and the Si(100)1×1 structure is changed back to the reconstructed Si(100)2×1 with the Se forming a 2×1 structure. The models of Se(1×1)/Si(100)1×1 and of the Se(2×1)/Si(100)2×1 structures are given. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Silicon and other semiconductors, such as GaAs and InP, are well known for their potentially wide use in high speed electronics and long wavelength optoelectrical circuits [1,2]. They have also demonstrated great value, mainly in space technology, as solar cells (photovoltaics) [3]. Their efficiency, however, is reduced by electron, X-ray and γ -radiation damage [4–6]. To protect the semiconducting surfaces without reducing their efficiency, the above semiconductors are passivated. This is done by depositing thin dielectric films such as gallium sulfide, indium sulfide and sulfur on the

surfaces [7–10]. Sulfur, selenium and tellurium deposition on semiconducting surfaces proved to be of particular interest, not only for passivation purposes, but also for their theoretically predicted ability to remove the initial dimer reconstruction on the (100) surface of Si and Ge [11-21]. One report claims that adsorption of sulfur on clean $Ge(100)2 \times 1$ changes the 2 × 1 structure to 1 × 1. which is regarded as an ideal terminated surface [22] although, according to another study [23], the ideal terminated surface of $Ge(100)1 \times 1$ may not occur with the suppression of the 2×1 reconstruction upon S adsorption. Moriarty et al. [24] reported that room temperature adsorption of S resulted in the formation of an overlayer with an underlying Si(100) which retained the 2×1 reconstruction. They also mentioned that annealing of

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the S/Si(100)2×1 surface to 325° C led to the desorption of the sulfur overlayer, and the appearance of the coexisting $c(4 \times 4)$ and 2×1 surface reconstruction. Recent reported observations [13], however, suggest that adsorption of elemental S on Si(100)2 \times 1 initially forms a 2 \times 1 (hemisulfide) structure up to 0.5 ML. Subsequently, the surface changes from a 2×1 to a 1×1 (monosulfide) structure in the coverage range 0.5-1 ML. Higher amounts of deposited S lead to the formation of a second layer, whereas part of the S diffuses into the bulk of the Si substrate. Cakmak and Srivasta have, very recently, calculated the location of S atoms above the Si(100) surface, and their results were in excellent agreement with the above proposed models of the hemisulfide (2×1) and monosulfide (1×1) structures [25]. Bringans and Olmstead [26] investigated the Se/Si(100)2 \times 1 system with low energy electron diffraction (LEED) and ultraviolet photoelectron spectroscopy (UPS) measurements, where they concluded that, at elevated temperatures $(300^{\circ}C)$, Se forms SiSe₂. Annealing at higher temperatures (500-550°C) results in only a submonolayer of Se atoms remaining in bridge sites with a 1×1 structure, while with theoretical calculations the conclusion was drawn that both Se and S change the 2×1 reconstructed Si(100) surface to its 1×1 form [11,12,21]. Tellurium deposition on Si(100)2 \times 1 grows in a Stranski-Krastanov mode, and forms a 1×1 structure [15–20]. From the above discussion it is clear that additional study of the S, Se and Te on Si(100)2 \times 1 is necessary. In this contribution we investigate the adsorption of Se on $Si(100)2 \times 1$ at room and elevated temperatures by Auger electron spectroscopy (AES), LEED, thermal desorption spectroscopy (TDS) and work function (WF) measurements, in ultra high vacuum (UHV).

2. Experimental

The experiments were performed in a UHV chamber, equipped with AES, LEED, a quadrupole mass spectrometer for TDS, with a heating rate of $\beta = 15$ K/s, and WF measurements. For the latter measurements we used the diode method.

The uncertainty in the WF measurements was 0.02 eV. Elemental Se was evaporated by thermal dissociation of WSe₂ single crystal flakes enclosed in envelopes made by thin Ta plates which were heated by passing current. During dissociation of WSe₂ the W remained in the Ta envelope, while Se was evaporated through holes made at the edge of the envelope. By plotting QMS signal intensity versus time for both atomic and molecular Se, with a constant current running through the Ta envelope, and comparing the areas under these graphs we measured the atomic Se to be 30% of the total yield. The Si(100) single crystal substrate was cleaned by heating at 1300 K, while the temperature of the sample was measured by a Cr-Al thermocouple calibrated by an infrared pyrometer in a temperature range 900-1300 K. The estimation of the Se coverage on Si(100) surface was based on a correlation of LEED, AES and TDS measurements. The surface atomic density of 1 ML Se on Si(100) is considered to be equal to that of the outermost layer of Si: 6.8×10^{14} atoms/cm².

3. Experimental results

3.1. Auger measurements — LEED

Fig. 1 shows the peak to peak height (Ap-pH) of the Se (47 eV) and Si (91 eV) Auger peaks as a function of the number of Se doses deposited on the Si(100)2 \times 1 surface at room temperature (RT) and with subsequent heating in steps of 100 K. These measurements are shown in correlation with the corresponding observed LEED patterns. As seen in Fig. 1, the Ap-pH of the Se (47 eV) peak increases almost linearly with an increasing number of Se doses. Near the eighth dose of Se deposition the curve forms a break and the Se peak continues to increase linearly with a lower rate up to 15 doses of deposition. Above the fifteenth dose the Se peak height increases with an even lower rate. The Ap-pH of Si decreases in a similar manner, and the corresponding curve shows breaks at the eighth and fifteenth doses of Se deposition (Fig. 1). This behavior is characteristic of layer by layer growth [27]. LEED observations show that Se causes a weakening of the half



Fig. 1. Auger peak to peak height (Ap-pH) of Se (47 eV) and Si (91 eV) as a function of the number of Se doses deposited on the $Si(100)2 \times 1$ surface at RT and with subsequent heating in steps of 100 K.

order spots of the Si(100)2 \times 1 pattern. The latter disappear near the first break (eighth dose of Se deposition) of the Se Auger curve (Fig. 1), while the integer order spots become more intense, and the pattern changes to a good 1×1 configuration. Between the eighth and fifteenth doses of Se deposition the LEED pattern does not show any substantial change and the 1×1 configuration remains. Higher Se coverages cause a decrease in the intensity of the integer order spots. The latter disappear for deposited Se amounts higher than 24 doses, while the background of the pattern becomes almost completely dark (approaching zero). Subsequent heating (Fig. 1) causes a small increase of the Si Ap-pH, while the Se Ap-pH does not show any substantial change up to 800 K. The LEED pattern depicts the 1×1 configuration once again in the range 400-800 K. In the 900-1100 K temperature range the Se peak decreases rapidly, the peak of the Si substrate increases proportionally to this, while the 2×1 LEED pattern reappears near 1000 K. The 2×1 LEED pattern becomes sharper with increasing temperature up to 1300 K.

3.2. Work function measurements — LEED

Fig. 2 shows the work function changes of the $Si(100)2 \times 1$ surface during Se deposition at RT, and after heating up to 1300 K, in correlation with the LEED observations. The work function increases almost linearly with Se deposition up to eight doses of Se. The work function change, at eight doses of Se deposition, is 0.52 eV. Higher Se deposition causes a decrease of the work function by 0.07 eV. Subsequent gradual heating of the system causes an increase of the work function to



Fig. 2. Work function change of the $Si(100)2 \times 1$ surface during Se deposition at RT, and after heating up to 1300 K, in correlation with LEED observations.

its maximum value (0.52 eV) at 600 K (point A). Heating the system to even higher temperatures decreases the work function and the curve forms a knee at about 1000 K (point B). The work function value of this knee is very close to that of 0.5 ML of Se deposited at room temperature, while the LEED pattern changes from a 1×1 to a 2×1 configuration. Further heating causes a drastic decrease of the work function which passes through a minimum value (-0.08 eV) at 1200 K and reaches the work function of the clean Si(100)2 × 1 surface at 1300 K.

3.3. TDS measurements

Fig. 3 shows a series of thermal desorption spectra of Se (79 amu) after Se depositions on Si(100)2×1 surfaces. The heating rate for all spectra was 15 K/s and it was constant in the whole temperature range of 300–1300 K. For an amount less than or equal to eight doses of Se the spectrum gives a peak β_1 at 1125 K. For Se coverages greater than the eighth dose, the spectrum shows a second peak β_2 of Se at a lower temperature of 1010 K, and finally a third Se peak β_3 at the relatively low temperature of 610 K. The first two peaks, from highest to lowest energy, correspond respectively to the thermal desorption of the first and second layers of Se on Si(100)2×1. The third peak represents added Se dosage corresponding to a third disordered layer of Se bonded with Si, by diffusing into the bulk or by drawing the Si out. It should be noted that the SiSe TD spectra consisted of the same peaks with approximately the same intensities as the aforementioned TD spectra for Se, and are not shown here. Fig. 4 shows a series of thermal desorption spectra of $SiSe_2$ (186 amu) after Se depositions on the Si(100) surface. As is seen in this figure, the SiSe₂ thermal desorption spectrum initially shows a single peak at 990 K for Se depositions above eight doses. At relatively very high Se coverages (greater than 25 doses), new broad peaks appear at about 600 K. These low temperature peaks increase with greater amounts of deposited Se.

Fig. 5 shows the thermal desorption spectrum of SiSe (107 amu), after Se deposition on the Si(100)2×1 surface, compared with those of Se (79 amu) and SiSe₂ (186 amu). The SiSe thermal desorption spectrum has two peaks. The high energy peak coincides with the Se peak β_1 at 1125 K for Se coverages equal to or less than eight doses. For Se deposition higher than eight doses this peak saturates and a second peak appears at 1010 K which coincides with the low energy Se peak β_2 . The intensity of this new SiSe (107 amu) double peak increases continuously with Se deposition. Selenium deposition higher than 15 doses



Fig. 3. A series of thermal desorption spectra of Se (79 amu) after Se deposition on $Si(100)2 \times 1$ surfaces. The numbers next to the curves indicate dosage.

causes the appearance of a third, low intensity, wide peak at about 600 K (not shown here).

4. Discussion

The first issue which needs to be addressed is the determination of Se coverage. The Auger measurements, according to Fig. 1, indicate that Se on Si(100)2 × 1 grows in a layer by layer mode [27]. The first layer is completed near the eighth dose of Se deposition when the first Auger break occurs, and the 1 × 1 LEED pattern appears. The TDS measurements of this study show, in addition, that up to the eighth dose of Se on Si(100), only Se and SiSe are detected. SiSe₂ is initially detected in the TDS measurements, on the other hand, after



Fig. 4. A series of thermal desorption spectra of SiSe₂ (186 amu) after Se deposition on Si(100) 2×1 surfaces. The numbers next to the curves indicate dosage.



Fig. 5. Thermal desorption spectrum of SiSe (107 amu), after Se deposition on the Si(100)2 × 1 surface, compared with those of Se (79 amu) and SiSe₂ (186 amu) at 20 doses of Se.

the twelfth dose (Fig. 4). The WF increases linearly up to the eighth dose, as well. This linear behavior of the work function curve is a clear indication of a constant dipole moment, which in turn indicates that the sites occupied by the Se on the Si substrate are all structurally similar surface sites up the eighth dose. Combining the above information, we may conclude that, at the eighth dose of Se, one Se adatom corresponds to one Si atom on the substrate's outermost layer. We may conclude, therefore, that at the eighth dose the first layer of Se is completed with a coverage of 1 ML (6.68×10^{14} atoms/cm²), which is consistent with the Auger measurements. Near the completion of the first Se layer the LEED pattern gradually changes from a 2×1 to a 1×1 configuration. The adsorption of elemental Se at room temperature, in other words, causes the transition of the reconstructed Si(100)2 \times 1 surface to its original bulk terminated $Si(100)1 \times 1$ state. The restoration of the 1×1 structure can be explained by the adsorption of Se atoms on the bridge and cave sites which cause the break of the Si-Si dimer bonds. This model is consistent with those proposed from previous experimental measurements of S and Te, on $Ge(100)2 \times 1$ and on $Si(100)2 \times 1$ [13,20,26,28], and via theoretical calculations [11,21]. Although the most likely sites to initially attract divalent Se adatoms are the dimer bridge sites, this analysis is not conclusive from the data in this study. The clarity of the 1×1 LEED pattern at a 1 ML Se coverage, however, points to an ordered 1×1 overlayer. Fig. 6b shows a side-view schematic, while Fig. 7b shows the topview schematic of 1 ML of the Se(1×1) structure on a Si(100)1 × 1 surface.

The second monolayer amount of Se is deposited between the eighth and sixteenth doses. The linearity of the Auger curve between breaks (Fig. 1) is an indication that this amount forms an even layer. Between the completion of the first and the second Se layer, the 1×1 pattern remains unaltered. This occurrence may lead to the conclusion that the Se atoms of the second layer are also arranged in a 1×1 structure. The lowering of the work function for Se coverage above 1 ML (Fig. 2), however, suggests that the deposited Se above 1 ML may be submerged into the bulk just under the surface layer of the Si. It should be emphasized that the second monolayer of Se,



Fig. 6. Side-view schematic of (a) clean Si(100)2×1, (b) 1 ML of Se with the (1×1) structure on the Si(100)1×1 substrate, (c) 2 ML of Se on Si(100)1×1, (d) 0.5 ML of Se with the 2×1 structure on Si(100)2×1 after heating the Se(1×1)/Si(100)1×1 surface to 1000 K.



Fig. 7. Top-view schematic of (a) clean Si(100)2×1, (b) 1 ML of Se with the (1×1) structure on Si(100)2×1 after heating the Se(1×1)/Si(100)1×1 surface to 1000 K.

according to these observations, is an even underlayer with a periodic 1×1 arrangement. The apparent periodicity and even distribution of the underlayer, and the appearance of the β_2 TD peak after the eighth dose (which is shown further in the text to maintain a binding energy of a covalent nature) point to the likelihood of Se insertion into the Si—Si bonds. We cannot, therefore, exclude the possibility that the two layers of Se may actually form a double-layer Si—Se lattice compound with the substrate. A possible model to explain the double $Se(1 \times 1)$ layer configuration on the $Si(100)1 \times 1$ surface is shown by the sideview schematic in Fig. 6c. The top view appears the same as that in Fig. 7b, since the Se atoms of the second layer are correspondingly under those of the first.

The TD measurements in Fig. 3 indicate that Se is deposited on Si(100)2 × 1 in three adsorption states: β_1 , β_2 and β_3 . Considering the desorption energy E_d to be equal to the binding energy E_b of an adsorbate, we can estimate the latter with the use of Redhead's equation [29]:

$$E_{\rm d} = RT_{\rm p}[\ln(vT_{\rm p}/\beta) - 3.64] \tag{1}$$

where T_p is the temperature, $\beta = 15$ K/s is the constant heating rate, R is the gas constant and vis the pre-exponential factor which for Si substrates is 10^{13} s⁻¹. The binding energies which correspond to β_1 , β_2 and β_3 desorption states are 2.97 eV/atom, 2.67 eV/atom and 1.58 eV/atom, respectively. The relatively high binding energies and the formation of the SiSe and SiSe₂ compounds suggest a covalent bond between Se and Si. As shown in Fig. 5, the two TD peaks formed by the first two Se monolayers are detected by the mass spectrometer as SiSe as well as Se. This may indicate that the β_1 and β_2 thermal desorption peaks are formed from the possible dissociation of SiSe₂. Whether or not this actually occurs, the aforementioned double layer of Se (at 2 ML) (Fig. 6c) fulfils the SiSe₂ stoichiometry with the Si substrate, and maintains a different covalent binding state from that of the Si–Se bond up to a coverage of 1 ML.

Above the sixteenth dose Auger data indicates the formation of a third Se layer. Adsorption of Se above 2 ML causes a gradual disappearance of the integer order spots of the Si(100)1 × 1 structure while the background becomes almost completely dark. For Se coverage above 2 ML (Figs. 3 and 5), TDS gives the β_3 low energy peak of Se and that of SiSe₂ at about 600 K. The presence of the latter SiSe₂ may indicate that some adsorbed Se atoms either diffuse into the bulk, bonding loosely with Si atoms, or reside on the surface where they cause a diffusion of Si atoms from the bulk to the surface.

Our data clearly shows a dominating $SiSe_2$ peak at 990 K, distinct from peaks β_1 and β_2 . It is most

likely that the Si-Se covalent bonds at the completion of the second monolayer, when the SiSe₂ stoichiometry is fulfilled, maintain the binding energy represented by the β_2 TD peak (Fig. 3). We may thus consider the resulting double layer Si/Se surface lattice structure to be a substratedependent SiSe₂ pseudocompound. The higher binding energy of TD peak β_1 probably corresponds to the stoichiometry of a coverage of 1 ML or less. Above the second monolayer the β_2 peak continues to increase, which indicates (in accordance with work function and Auger measurements) that Se continues its bonding with Si below the second layer. The β_2 peak saturates at 20 doses (an equivalent of 2.5 ML). It is at this point that the 990 K SiSe₂ begins to dominate. It must be noted, however, that the SiSe₂ detected at a coverage above 2 ML at 990 K may actually form during the thermal desorption process, where sufficient activation energy through heating is provided. This high coverage (above 2.5 ML) is thus marked by Se diffusion into the bulk, which may contribute (with the loosely bound Se and SiSe₂) to the disappearance of the 1×1 LEED pattern. The Si-Se double lattice layer (with SiSe₂ stoichiometry) nevertheless remains over the disordered layers as a crystal lattice 'crust', and is again 'revealed' upon heating (as explained below).

Gradual heating of more than three equivalent monolayers of Se on Si(100)2 \times 1 initially causes the desorption of the loosely bound SiSe₂ overlayer and the reappearance of the 1×1 pattern. The work function, at this point, reaches its maximum value of 0.52 eV, corresponding to a 1 ML room temperature coverage, while Auger measurements indicate an equivalent coverage over 3 ML. The apparent inconsistencies in data give rise to the question of how LEED and WF data can indicate a clear 1×1 surface restoration at 1 ML when both TDS and AES data clearly substantiate the presence of at least 3 ML of Se on the Si(100)1 \times 1 surface. To reconcile the above data one need only consider that LEED and WF give information relating mostly to the state of the sample surface, while AES and TDS show the total amounts of the adsorbate. We believe, therefore, that the most likely answer is that at 600 K 1 ML of Se remains on the surface, suppressing the reconstruction,

while the rest resides in the substrate bulk (Figs. 6b and 7b).

Further heating (to 990 K) removes the bulk SiSe₂ (corresponding to the Fig. 4 TD peak) and brings the coverage to 2 ML, according to AES data. LEED observations show a disordered surface state most likely caused by the desorption of the bulk SiSe₂, while the WF curve becomes nonlinear. At about 1000 K (approximately equal to the desorption temperature of peak β_2), the LEED pattern shows a strong 2×1 pattern, and the WF curve exhibits a characteristic knee as the AES plot indicates 1 ML. The corresponding room temperature coverage for the WF value at this (point B) is 0.5 ML. Data here indicates that an amount of 1 ML of Se is distributed on (and in) the substrate, while it maintains the strong covalent bonding which characterizes TD peak β_1 . The WF information indicates a 0.5 ML Se coverage on the substrate surface, distributed in such a way as to allow the observation of a clear 2×1 LEED pattern. We believe that, at this point, the $Si(100)2 \times 1$ reconstruction is reproduced with the Se atoms bound through the dangling bonds to the two Si atoms of each dimer. This is consistent with the fact that Se is divalent. When all the dimer bridge sites are filled, moreover (on the $Si(100)2 \times 1$ surface), the maximum surface coverage is 0.5 ML. The model of $Se(2 \times 1)$ on $Si(100)2 \times 1$ is shown by the side-view and topview schematics in Figs 6d and 7c, respectively. We can further support the formation of the $Se(2 \times 1)$ structure on $Si(100)2 \times 1$ by correlating it with the work function variation in the 600-1000 K temperature range between the points A and B in Fig. 2. Fig. 8 shows the work function variation during heating the Se (1×1) /Si(100)1 × 1 surface structure from 600 K (point A) to 1000 K (point B) where the above structure has changed to the Se(2 \times 1)/Si(100)2 \times 1. The sizes of the Se and Si atoms in this figure are considered in proportion to their real size with the Se-Si bond being covalent, as shown previously. The covalent radii of Se and Si are 1.16 and 1.11 Å, respectively. The dipole lengths of the dipole moments which correspond to the structures at the points A and B (Fig. 8) are d=1.6 and 2.1 Å, respectively. The work function value for a coverage Θ of an



Fig. 8. The work function variation during heating of the $Se(1 \times 1)/Si(100)1 \times 1$ surface structure from 600 K (point A) to 1000 K (point B) where the above surface structure has changed to the $Se(2 \times 1)/Si(100)2 \times 1$ configuration.

adsorbate on a substrate is given by

$$\Phi = 2\pi P N_{\rm s} \Theta = 2\pi q N_{\rm s} \Theta \tag{2}$$

where P = qd is the electric dipole moment, N_s the density of the atoms in the outermost layer of the adsorbate [30] and q the charge of each adsorbed atom. The charge q remains constant due to the covalent nature of the Si—Se bonds. If the d= 16 Å remains constant and the surface Θ changes from 1 to 0.5 ML, the Φ should decrease linearly to a value lower than that at B. Based on the above argument, the only way to explain the gradual slope decrease of the Φ curve between A and B may be attributed to an increase of the dipole length to d=2.1 Å, which is due to the formation of a Se(2 × 1) structure on Si(100)2 × 1, as shown in Figs. 6d and 7c.

From our LEED observations, there is no clear indication of Se(2×1) formation during Se deposition at RT such as for S on Si(100)2×1 [13]. The strong binding energy of Se on Si(100)2×1 (E_b =2.97 eV/atom) is greater than that of S on Si(100)2×1 (E_b =2.24 eV/atom) [13], and probably restricts the mobility of the Se atoms so that their diffusion onto the dimer bridge sites is less

than that of S on the same surface. This mobility is, most likely, obtained by heating which provides the required activation energy for Se atoms to rise up to the bridge sites.

5. Conclusions

In this paper we study the adsorption of elemental Se on the Si(100)2 \times 1 surface at room and elevated temperatures by LEED, AES, TDS and WF measurements. The adsorption of 1 ML of elemental Se at RT causes the transition of the reconstructed Si(100)2 \times 1 surface to its original bulk terminated $Si(100)1 \times 1$. The deposited monolayer of Se forms a 1×1 structure on $Si(100)1 \times 1$ by breaking the Si-Si dimer bonds. The Si-Se bond is strong ($E_{\rm b}$ =2.97 eV/atom), suggesting a covalent bonding which results in the formation of a SiSe surface compound. Above 1 ML and up to the completion of 2 ML, deposited Se is submerged into the bulk near the surface of the Si(100)1 \times 1 substrate. This process results in the formation of a SiSe₂ stoichiometry with a binding energy $E_{\rm b} = 2.67 \, {\rm eV}/{\rm atom}$. With further deposition, the Se atoms are loosely bound on top of the SiSe₂ layer ($E_b = 1.58 \text{ eV}/\text{atom}$), which may continue its formation through a diffusion of Si atoms from the bulk to the surface. The following heating procedure caused the gradual desorption of Se (in SiSe or SiSe₂ compounds) up until 1000 K where the Se surface coverage becomes 0.5 ML and the Si(100)1 × 1 structure changes back to the reconstructed Si(100)2 × 1 surface. The models of clean Si(100)2 × 1, Se(1 × 1)/Si(100)1 × 1, and of the Se(1 × 2)/Si(100)2 × 1 structures are given in Figs. 6 and 7.

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