THE FORMATION OF A SURFACE IODIDE ON Ni(100) AND ADSORPTION OF I₂ AT LOW TEMPERATURES

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Iodine adsorption on clean Ni[100] has been investigated using low energy electron diffraction (LEED) and Auger electron spectroscopy (AES). At temperatures below 340 K a saturated surface of adsorbed iodine atoms in a $c(2 \times 2)$ structure is observed. Adsorption of iodine on clean Ni(100) at temperatures in exces of 370 K forms a structure identified as a single layer of the layered compound NiI₂ on the metal substrate Solid iodine is shown to grow epitaxially on both the $c(2 \times 2)$ chemisorbed surface and the surface iodide at temperatures less than 185 K. Heating to 185 < T < 226 K leaves a physisorbed molecular iodine layer, while on returning to room temperature the original $c(2 \times 2)$ or iodide is restored.

1. Introduction

In a previous paper [1] we discussed the dissociative adsorption of iodine on Ni(100) at room temperature and above, to form a chemisorbed adlayer. In this paper we describe the formation of an incommensurate surface structure on Ni(100) consistent with the formation of a surface iodide, and the adsorption of molecular iodine on this and the $c(2 \times 2)$ chemisorbed adlayer at low temperatures.

The high temperature, low coverage, $I/Ni{100}$ surfaces studied previously [1] exhibited the variable non-coincident structures common to many halogen/metal adsorption systems (e.g. ref. [2]). The Ni{100} surface also showed a slow but significant uptake of iodine beyond the initial saturated $c(2 \times 2)$ surface. We show here that this was due to the formation of a single layer of nickel di-iodide on the surface.

Formation of bulk copper(I) bromide has been observed by Richardson and Sass on Cu(100) [3] while the transformation of a chemisorbed adlayer to a bulk chloride was observed by Kitson and Lambert on Ag(100) [4]. Bulk halide formation in UHV apears to be sensitive to substrate crystallography. Both chloride [5] and iodide [6] are formed on Au(111), but no bromide formation occurs on Au(100) [7]. Recently it has also been shown [8] that bulk CuI grows epitaxially on Cu(111) due to the close matching of I–I distances in the (111) plane of CuI and the $(\sqrt{3} \times \sqrt{3}) R30^\circ$ adsorbate structure. Similar arguments

are used in this work to explain the growth of NiI₂ on Ni(100). Adsorption of I₂ on the cooled $c(2 \times 2)$ and iodide surfaces showed the existence of physisorbed molecular I₂ at temperatures well above that required

2. Experimental

for condensation.

The apparatus consisted of a stainless steel UHV chamber of base pressure 5×10^{-9} Pa (1 Torr = 133.3 Pa). Conventional three grid optics (VG Scientific Ltd.) were used for LEED display and AES. The Ni(100) crystal was cut, polished, and after insertion in vacuum, cleaned by cycles of argon ion bombardment and annealing to ≈ 1000 K. Carbon, oxygen, sulphur and phosphorus were undetectable (< 2% of a monolayer). Iodine could be leaked into the chamber at pressures up to 1×10^{-4} Pa, the purity being checked with a quadrupole mass spectrometer.

Auger electron spectra were taken by modulating the sample with a 5 V RMS sinusoidal signal while the second derivative of the collector current was recorded using lock-in techniques. The crystal and crystal holder were cooled by a length of copper braid attached to a reservoir of liquid nitrogen. The sample could be cooled to 140 K in approximately 45 min.

3. Results

Two different, stable overlayer structures were normally formed by iodine adsorption on the clean Ni(100) at room temperature. Each structure was investigated individually and then used as the substrate for additional adsorption of molecular iodine at low temperatures.

The first structure, characterised by a sharp $c(2 \times 2)$ LEED pattern, was formed by exposing the clean Ni{100} surface at room temperature (below 340 K) to iodine at $\sim 2 \times 10^{-5}$ Pa for 300 s.

The second structure was formed by exposing the clean Ni(100) surface at a temperature in the range 370 to 1000 K to an iodine pressure of ~ 10^{-4} Pa, followed by cooling in the iodine atmosphere to room temperature. A sharp well defined LEED pattern, fig. 1, was produced. It will be shown later that this LEED pattern corresponds to the formation of a single incommensurate layer of nickel di-iodide, labelled structure I. This surface iodide structure remained stable when heated in vacuum to temperatures below 470 ± 20 K. At temperatures in excess of 490 K the LEED pattern changed to a $(-1 - \frac{1}{4} \frac{1}{4 \tan \alpha})$ structure, fig. 2, identical to that formed by heating the $c(2 \times 2)$ iodine surface to the same temperature and previously interpreted as being due



Fig. 1. Incommensurate surface iodide structure I on Ni(100). Beam energy 51 eV.

to a variable size incommensurate chemisorbed overlayer [1].

Two additional complex structures were observed at room temperature after very slow adsorption of iodine at low pressure onto the Ni(100) over several days. Each was found to have the same iodine to nickel Auger peak to peak height ratio as the incommensurate iodide structure, but these new structures had coincident nets. These will be labelled commensurate structures II, fig. 3 and III, fig. 4. It will be shown that these structures can be reconciled with slight distortions of the iodide structure I.



Fig. 2. The $\begin{pmatrix} 1 & l/(\tan \alpha) \\ -1 & l/(\tan \alpha) \end{pmatrix}$ dissociatively chemisorbed iodine structure formed by heating structure I to 490 K. Beam energy 32 eV.



Fig. 3. Surface iodide structure II on Ni(110). (a) Beam energy 31 eV. (b) Schematic of (a). (c) Beam energy 23 eV. (d) Schematic of (c).

Adsorption of iodine on the $c(2 \times 2)$ chemisorbed iodine surface and the incommensurate surface iodide at temperatures T < 160 K, was monitored by AES. After large exposures to iodine ($\simeq 0.1$ Pa s, where 1 Pa s = 7500 L) the iodine Auger peak intensity (seen as a poorly resolved doublet at 511 and 520 eV) reached a limiting value due to condensed multilayers of iodine; the high energy nickel Auger peaks (716, 783 and 848 eV) were reduced to the noise level (attenuated by > 30 times) while the low energy nickel Auger peak was attenuated by approximately six times. This observation would appear to be at variance with the energy dependence of the inelastic scattering mean-free-path displayed by "universal curves" [9] and we are unable to account for this discrepancy.

Fig. 5 shows a plot of iodine Auger peak to peak intensity (as a percentage



Fig. 4. Surface indide structure III on Ni(100). (a) Beam energy 27 eV (b) Schematic of (a). (c) Beam energy 27 eV. (d) Schematic of (c). (e) Beam energy 30 eV (f) Schematic of (e).



Fig. 5. Adsorption curves for I₂ on chemisorbed $c(2 \times 2)$ surface (lower curve) and surface iodide structure I (upper curve) at T < 160 K. A 100% iodine Auger signal is equivalent to multilayer condensation of iodine.

of the saturated iodine Auger signal) versus exposure during the early stages of adsorption. On both the chemisorbed $c(2 \times 2)$ surface and the surface iodide, a rapid initial rise is followed by a much slower increase. LEED observations show a reasonable well ordered pattern for the multilayers of iodine formed after large exposures, fig. 6.



Fig. 6. (2×4) structure for multilayer condensation of I₂ on the $c(2 \times 2)$ substrate. Beam energy 41 eV.



Fig 7. Desorption of solid iodine from the $c(2 \times 2)$ and surface iodide structure I substrates. $c(2 \times 2)$ substrate: (\mathbf{v}) iodine Auger peak height, ($\mathbf{\Phi}$) nickel Auger peak height; surface iodide substrate: ($\mathbf{\Phi}$) iodine Auger peak height. (\mathbf{H}) nickel Auger peak height.

Following adsorption, each surface was allowed to return to room temperature over the period of about 1 h. During this period AES spectra were taken in the regions of the nickel and iodine peaks. The exposure of the sample to the 2 keV primary electron beam was kept to a minimum. Fig. 7 shows plots of iodine (511 and 520 eV) and nickel (716 eV) Auger peak to peak heights versus temperature for desorption from the chemisorbed $c(2 \times 2)$ and surface iodide substrates. The iodine Auger peak undergoes an abrupt drop and the nickel Auger peak an abrupt rise at approximately 185 K. We identify this as due to desorption of multilayers of iodine from the surface. At approximately 226 K there is another drop in the iodine, and increase in the nickel, Auger peak heights. This is identified as desorption of a physisorbed layer of iodine which can exist on either substrate. On return to room temperature the substrate surface was found to be unchanged, as monitored by LEED and AES.

4. Interpretation and discussion

4.1. Room temperature adsorption; surface iodides

The diffraction pattern from the incommensurate surface iodide structure I is shown in fig. 1 and a schematic representation is shown in fig. 8. The arrows drawn in fig. 8 are to indicate that there was a small variation in position from one structure to the next.



Fig. 8. Real and reciprocal space nets for surface iodide structure I. Open circles show Ni(100) lattice points; closed circles the NiI₂ lattice points. Reciprocal space shows beams for both orientations and double diffraction.

We refer to the periodicity of the Ni(100) surface as the *a* net with unit mesh vectors a_1 and a_2 . The overlayer net is referred to as the *b* net with unit mesh vectors $_1b_1$ and $_1b_2$; the Roman pre-subscript denotes which structure is being described. The LEED pattern for structure I is described by $_1b_1^*$ which terminates at the (1/2, 1/2) position, and $_1b_2^*$ which terminates along CD (fig. 8). The real space structure is also shown in fig. 8 in which all the overlayer lattice points lie along $\langle 11 \rangle$ directions. The structure shown in fig. 8 is related to the substrate mesh by the matrix

$(1-1/(\tan\theta))$	$-1-1/(\tan\theta)$
$(2/(\tan\theta))$	$2/(\tan\theta)$

where $\theta \sim 61^{\circ}$ gives the unit mesh dimensions of $_{1}b_{1} = 4.0$ Å and $_{1}b_{2} = 3.9$ Å.

Bulk nickel di-iodide, NiI₂, has the cadmium chloride structure, consisting of an hexagonal prism of base 3.892 Å with a height of 19.634 Å, containing three formula units [10]. The structure is layered, each layer consisting of two layers of iodine atoms with nickel atoms occupying the octahedral interstices. This leads us to suggest that structure I is a single layer of nickel di-iodide (hence ~ 6.5 Å thick), fig. 12. Relative to bulk NiI₂, the unit mesh of structure I involves a slight distortion (to an included angle of 61° rather than 60°) and a linear expansion of the vectors by about 4.5%. The iodine and nickel Auger peak heights for structure I, fig. 7, are also consistent with the above model (see appendix).



Fig 9 Real and reciprocal space nets for surface iodide structure II. Reciprocal space diagram shows beams for both orientations

The surface iodide was destroyed by heating to 490 K, leaving a dissociatively chemisorbed iodine layer (characterised by the LEED pattern in fig. 2), which is found to have a coverage $\Gamma = 0.45$ [1] *. It is interesting to note that this is very close to the iodine atom coverage per layer within the original surface iodide ($\Gamma = 0.44$): we therefore speculate that the surface iodide may decompose by desorption of NiI and retention, and rearrangement, of the iodine layer adjacent to the Ni(100) substrate. Bulk growth of NiI₂ was not observed on Ni(100). This may be explained by the high vapour pressure of NiI₂, about 5×10^{-8} Pa [17] at the temperatures necessary for its formation, 370 < T < 490 K.

Two separate coincident structures were also observed, structures II and III, both exhibiting the same iodine to nickel Auger peak to peak height ratio as found for the incommensurate surface iodide structure I. The LEED pattern for the first of these, structure II, is shown in fig. 3 and schematically in fig. 9. The coincidence net $(_{11}c)$ is related to the substrate net by the matrix $(\frac{5}{3}, \frac{3}{5})$ (Wood notation $(\sqrt{34} \times \sqrt{34})$ R arctan(3/5)). There are two domain orientations for this structure. Fig. 9 also shows an overlayer net $(_{11}b)$ which coincides periodically with the Ni(100) substrate to form the $(\frac{5}{3}, \frac{3}{5})_{11}c$ net (fig. 9 and table 1). $_{11}b_1$ and $_{11}b_2$ are of equal length, 3.99 Å, and subtend an included angle of 61.93°. This therefore is also consistent with a layer of nickel di-iodide which has undergone a slight expansion and rotation, in this case enabling it to form a coincident structure. It should be noted that the lattice points of the *b* net lie along $\langle 11 \rangle$ rows.

^{*} Γ is a surface concentration in units of adatoms per substrate unit mesh.

Table I						
Structure	b_1	b_2	Included angle, θ (deg)	f q	b Net matrix	c Net matrix
Bulk NiI ₂	3.892 Å	3.892 Å	60	1	E	ŧ
Structure I	$\left[\sqrt{2} / (\sin \theta)\right] a_1 $ (4.02 Å)	$\left[\frac{2\sqrt{2}}{(3.90 \text{ Å})}\right] a_1 $	61	$4^{1}_{4} \tan \theta$ (0.45)	$\begin{pmatrix} 1-1/(\tan\theta) & -1-1/(\tan\theta) \\ 2/(\tan\theta) & 2/(\tan\theta) \end{pmatrix}$	an a
Structure II	[(17√2)/15] a ₁ (3.99 Å)	[(17√2)/15] a1 (3.99 Å)	61.93	15/34 (0.44)	$\begin{pmatrix} 23/15 & -7/15 \\ 17/15 & 17/15 \end{pmatrix}$	$ \begin{pmatrix} 5 & \overline{3} \\ 3 & 5 \end{pmatrix} $ ($\sqrt{34} \times \sqrt{34}$)R arctan($3/5$)
Structure III	(√ <u>314</u> ∕11)(<i>a</i> 1 (4.01 Å)	(√ <u>1250</u> ∕22)(a,) (4.00 Å)	61.39	11/25 (0.44)	$\begin{pmatrix} 17/11 & -5/11 \\ 25/22 & 25/22 \end{pmatrix}$	$\begin{pmatrix} 7 & \overline{5} \\ 3 & 5 \end{pmatrix}$



Fig. 10. Real and reciprocal space mesh for surface iodide structure III. Reciprocal space diagram shows beams for all four orientations.

The LEED pattern of structure III is shown in fig. 4 and schematically in fig. 10. The corresponding coincidence net is defined by the matrix $\begin{pmatrix}7 & 5\\3 & 5\end{pmatrix}$. The translation vectors for an associated _{III}**b** net have lengths of 4.00 and 4.01 Å, and the included angle is 61.39° (table 1). The lattice points again lie along $\langle 11 \rangle$ rows. Structures II and III may now be seen as slight distortions of the incommensurate surface iodide structure I, which allow it to come into coincidence with the Ni(100) surface.

4.2. Low temperature adsorption

The LEED pattern observed for multilayers of iodine condensed on a $c(2 \times 2)$ surface is shown in fig. 6 and schematically in fig. 11. It may be indexed as a (2×4) structure and can be explained by the epitaxial growth of iodine on the $c(2 \times 2)$ (or on the surface iodide) surface.

Solid iodine has a layered structure with an orthorhombic unit cell; the projection of the unit cell is a rectangle of dimensions 4.69 Å by 9.78 Å at 110 K [11]. The (2×4) unit cell on Ni(100) has the dimensions 4.97 Å by 9.93 Å at 123 K. Epitaxial growth of solid iodine therefore requires only slight distortion to match the (2×4) unit mesh. Fig. 11 illustrates this fit on both the $c(2 \times 2)$ and the incommensurate iodide structure. We note that all three iodide structures involve alignment along the $\langle 11 \rangle$ rows with very similar atom spacing, and thus a similar relationship arises for all these surfaces.



Fig. 11. Real and reciprocal space for the (2×4) structure of solid iodine. In real space the $c(2 \times 2)$ substrate net is shown thus ----- and the $\langle 11 \rangle$ directions along which the lattice points of structure I he, thus ----.

Note that the epitaxial layer of solid iodine has two glide planes (space group p2g) which should lead [12] to systematic absences in the LEED patterns provided the incident beam lies in either the (001) or (010) planes. A verification of this awaits further study.



Fig. 12. A single layer of the bulk NiI₂: (\bullet) Ni atoms, (\bigcirc) I atoms.

Desorption of the solid iodine phase from the surface at approximately 185 K is consistent with bulk evaporation; the vapour pressure of solid iodide at 185 K is $\sim 4 \times 10^{-5}$ Pa [13] while the background pressure during desorption was $\sim 10^{-6}$ Pa.

The physisorbed layer of iodine which exists on both the $c(2 \times 2)$ and surface iodide surfaces attenuates the nickel Auger peaks from both substrates by the same amount (see appendix), indicating that this layer has the same concentration on both substrates. Further analysis shows that the atomic concentration of iodine within the physisorbed layer is $\Gamma = 0.32 \pm 0.03$ (see appendix). The activation energy for desorption of this physisorbed phase can be estimated using Redhead's equation [14], assuming first order kinetics, as 65 kJ mol⁻¹ ± 10%; this error range covers possible errors in the heating rate and values for the pre-exponential ν in the range 10^{12} to 10^{14} s⁻¹. This lies close to the upper limit of physisorption energies which is usually considered to be ~ 60 kJ mol⁻¹.

If we assume that the iodine in this layer is molecular, then the experimental atomic coverage ($\Gamma = 0.32 \pm 0.03$) yields an area per molecule of 39 ± 4 Å² on the surface. This high density may indicate the presence of a two-dimensional liquid. Following the method of De Boer [15] the two-dimensional equation of state for a Van der Waals fluid is



$$\left(F+a_2/A^2\right)\left(A-b_2\right)=RT,$$

Fig. 13. Plots of F versus A at T = 350, 226 and 200 K for the two-dimensional Van der Waals equation of I₂. The approximate level of condensation for 226 and 200 K is indicated. The A scale $(Å^2)$ is logarithmic

where F is the surface force, A is the area, and a_2 and b_2 are the two-dimensional Van der Waals constants. These constants can be calculated from the molecular diameter, 4.3×10^{-10} m, and the critical temperature, 819 K, for iodine. In fig. 13 three plots of this equation are shown for T = 200, 226 and 350 K. It can be seen that condensation will occur within the two-dimensional layer for areas per molecule of less than 10^4 Å^2 for temperatures between 200 and 226 K. The condensed phase has a coverage of ~ 36 Å² per molecule which agree well with our experimental value of $39 \pm 4 \text{ Å}^2$ per molecule. The physisorbed layer is therefore compatible with a two-dimensional molecular liquid.

We note that the physisorbed layer, with $\Gamma = 0.32$, is characteristic only of the desorption sequence and, indeed, its properties have been related to the higher temperatures used in desorption. The *adsorption* of iodine on the $c(2 \times 2)$ and iodide substrates shows no obvious break in sticking factor at this coverage although there is a reduction in sticking at high coverage. It seems likely that this occurs at the completion of a $\Gamma = 0.5$ layer which would form the first layer of the (2×4) bulk iodine structure.

5. Conclusions

In the temperature range T < 340 K iodine adsorbs dissociatively on Ni(100) to form a $c(2 \times 2)$ chemisorbed layer. For temperatures between 370 and 470 K iodine reacts with the surface to form a surface nickel di-iodide consisting of a double layer of iodine atoms with nickel atoms in the octahedral interstices. Formation of bulk NiI₂ is not observed under UHV due to the high vapour pressure of NiI₂ at the temperatures necessary to form the bulk halide. One incommensurate and two coincident surface iodide structures are observed, all closely related.

For temperatures between 185 and 226 K a physisorbed layer of molecular iodine is formed on both the $c(2 \times 2)$ and surface iodide surfaces. From the concentration of iodine in the physisorbed phase, we propose that this layer is a two-dimensional liquid. At temperatures below 185 K adsorption of iodine on each overlayer leads to epitaxial growth of solid iodine. This growth occurs with the basal plane of the layered solid iodine parallel to the Ni{100} surface.

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Appendix. Coverage determination using Auger electron spectroscopy

In this short appendix we will discuss the methods used to determine the overlayer coverages of the various structures observed which have been used in the interpretation and discussion of the main text. Table 2 shows the main numerical results used, the I and Ni Auger signals being arbitrarily normalised to unity for one particular structure for each species as shown. In all the analysis we take as the fixed point the fact that the $c(2 \times 2)$ structure should correspond to one half of a monolayer of iodine ($\Gamma = 0.50$). We also note that the inter-adsorbate atom spacing in this structure (3.52 Å), from consideration of atomic radius, corresponds essentially to the largest coverage possible in a single layer of iodine atoms (although close packing could conceivably increase this by 15%).

Physisorbed layer. We note first that the attenuation of the nickel Auger signal associated with the addition of the physisorbed layer is by a factor of 0.79 on the c(2 \times 2) substrate and 0.77 on the iodide substrate, indicating that these two physisorbed layers must have essentially the same iodine coverage. If we now assume that the I and Ni Auger signals occur at sufficiently similar energies (511, 520 and 716 eV) for this same attenuation coefficient to apply to the iodine signal from the iodine in the substrate (below the physisorbed layer), then we can readily calculate the iodine coverage in the physisorbed layer. Remembering that a normalised iodine signal of 0.33 corresponds to Γ of 0.50, this calculation for the c(2 \times 2) substrate therefore gives

 Γ (physisorbed) = (0.50/0.33)(0.48 - 0.33 × 0.78) = 0.34.

A similar calculation for the physisorbed layer on the iodide substrate gives Γ (physisorbed) = 0.29. We therefore use, for the purpose of discussion in the text, a coverage of $\Gamma = 0.32$ with an apparent error of about 10%.

Incommensurate iodide. The substantially greater I Auger yield from the

Structure	I $M_5N_{45}N_{45} / M_4M_{45}N_{45}$ (511, 520 eV)	N1 $L_3 M_{23} V$ (716 eV)
	0.33	1.00
$c(2 \times 2)I + physisorbed layer$	0.48	0.79
Incommensurate iodide	0.47	0 91
Incommensurate iodide + physisorbed layer	0.56	0.70
Multi-layer solid iodine on either substrate	1.00	0.00

Relative peak-to-peak Auger electron signals from various structures found by iodine adsorptions on Ni(100)

Table 2

iodide structure relative to the $c(2 \times 2)$ state makes it clear that this structure contains at least two layers of iodine. The fact that we have reconciled the $c(2 \times 2)$ plus physisorbed layer structure as being two layers in the previous section, and that the iodine Auger yield from this structure is essentially identical, leads to the view that the iodide probably also contains just two layers. In the main text we have proposed a specific two layer structure based on the similarity of the unit mesh to that of bulk NiI₂. We, therefore, wish to establish whether the observed Auger yields are consistent with this structure. The proposed structure (fig. 8) contains two identical layers of iodine, coverage $\Gamma = 0.44$, with a "sandwiched" nickel layer of the same coverage. The top iodine layer then must give an iodine Auger signal of $0.44 \times 0.33 / 0.50 = 0.28$, leaving a remaining signal of 0.19 to be reconciled with the attenuated lower layer. Our problem now is to establish some attenuation coefficient for the effect of this upper iodine layer, and the sandwiched nickel layer, on the Auger signal from the first layer. If we assume these combined overlayers have the same attenuation coefficient as the physisorbed layer of iodine alone (0.78)then the first layer ($\Gamma = 0.44$) would lead to an Auger contribution of 0.22. If, we assume that the attenuation by the top iodine layer is enhanced relative to that of the physisorbed layer by a linear scaling of their atom densities but still take no explicit account of the nickel layer, the new attenuation coefficient (0.70) leads to an Auger signal contribution from the first iodine layer of 0.195, in quite good agreement with experiment. Why we should be able to achieve this agreement with total neglect of the role of the sandwiched nickel layer is unclear. One could, of course, propose that no such nickel layer is present. However, the current understanding of the material dependence of inelastic scattering electron mean-free-paths is poor, and indeed there is certainly experimental evidence from the difference in attenuation in oxides relative to metals that inelastic scattering may be weaker in compounds than in elemental solids [16]. The Auger evidence, therefore, would appear to support the view that the iodide structure does, indeed, contain two iodine layers of approximately the correct density; while the iodine Auger data cannot cast any light on the density of the intermediate nickel layer, we note that the fact that the nickel Auger signal is significantly larger from the iodide structure than from the $c(2 \times 2)$ plus physisorbed state does support the view that this intermediate nickel layer is present.

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