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LETTER TO THE EDITOR

LEED study of mixed one-dimensional lead and thallium chains on Cu(100)

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Abstract. A LEED study has been carried out on mixed lead and thallium overlayers. The observed patterns are consistent with earlier chain models of the pure materials and indicate that the mixed systems contain areas of interpenetrating chains with interaction between chains of one material despite intervening chains of the other. For the samples with a thallium content exceeding 50%, there is evidence for the formation of chains in which the Peierls distortion observed in pure thallium overlayers is suppressed.

One-dimensional (1D) systems have long been of interest due to their exotic ground states, unique to 1D, and novel transport behaviour. One of the simpler aspects of 1D behaviour is the Peierls metal–insulator transition where, below the transition temperature, a superstructure or charge density wave (CDW) of wavelength $\lambda_{\text{CDW}} = 2\pi/k_F$ occurs along the chain accompanied by the appearance of a band gap at the Fermi level. Pseudo-1D overlayers, that is well separated atomic chains adsorbed on metal and semiconductor surfaces [1, 2] provide us with an opportunity to study approximations to ideal 1D systems using the powerful microscopic probes available in surface science.

Both lead and thallium adsorbed on Cu(100) form chain structures at sub-monolayer coverages and here we present the results of a LEED study of mixed lead and thallium overlayers. In the case of lead two alternative models have been proposed, that is, separate chains along the $\langle 10 \rangle$ direction of the Cu(100) surface [3] and interpenetrating chains along the $\langle 11 \rangle$ direction [4]. The data to be presented are consistent with the former model, which we adopt for the remainder of this report. Lead and thallium chains are particularly interesting systems for a comparative study since lead has a $6p^2$ outermost band that in an ideal 1D arrangement is filled, while thallium has a half-filled $6p^1$ outermost band. Thus lead chains are not expected to exhibit a Peierls distortion since $k_F = \pi/a$ giving $\lambda_{\text{CDW}} = a$, the atomic spacing. This is supported by the lack of evidence from LEED of any superstructure [3] along the observed $[\frac{1}{2} \frac{1}{2}]$ lead chain structure. Thallium, on the other hand, should undergo a lattice distortion corresponding to a dimerization and this has been observed at low temperature over a narrow coverage range [5]. The distorted chain structure has a $[\frac{1}{2} \frac{1}{2}]$ real space unit mesh corresponding

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to a superstructure which repeats every tenth thallium atom and a corresponding Fermi-level band gap of ≈ 0.25 eV. The Peierls distortion on thallium chains is rather fragile and can only be observed in overlayer structures that have a low commensurability with the substrate. Thus more commensurate thallium chain structures observed on Cu(100) [5] and Ag(100) [2] show no evidence for a CDW. Here we report a LEED study of mixed lead-thallium layers deposited on Cu(100) where each metal is deposited up to a coverage sufficient to produce the saturated chain structures described above over the surface not covered by the other material.

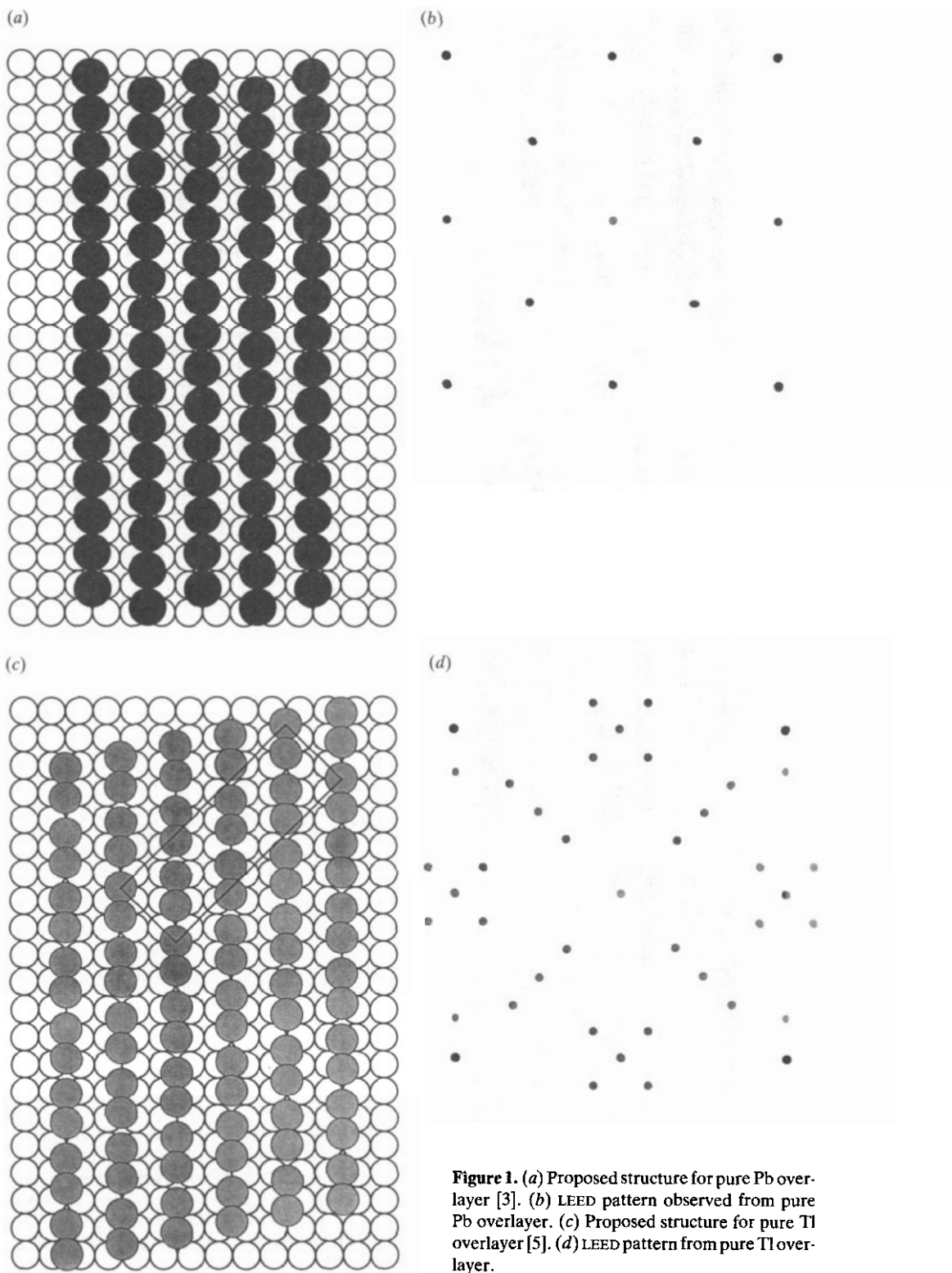
The experiments were performed in an ion-pumped μ -metal UHV chamber equipped with 4-grid LEED display optics that was also used as a retarding field analyser for recording Auger electron spectra. The overlayers were deposited from water-cooled Knudsen cell sources and the Cu(100) crystal was cleaned by cycles of Ar ion sputtering and annealing. The chamber pressure during evaporation was 2×10^{-10} mb.

The coverage was monitored by measuring the decay of the substrate MVV Auger signal as a function of evaporation time ($AS-t$). For both materials there is a kink in the $AS-t$ plot at the completion of the chain structures and the decay in the clean substrate signal at the kink was measured during the preparation of overlayers of the pure metals. For the mixed layers it was not possible to continuously co-evaporate and control the coverage with sufficient precision. Instead, the rate of decay of the Cu Auger signal was measured during a short deposition from each vapour source and the time required to form the correct proportion of the saturated chain structure of each material was thus determined. The deposition then proceeded as a series of (typically ten) short evaporations from each vapour source alternately. From the previously proposed models for the pure metals [3, 5] the linear density along lead and thallium chains is in the ratio 9:10. Thus the mixtures required to cover the surface with saturated chains in the area ratios 2:1, 1:1 and 1:2 are $Pb_{64}Tl_{36}$, $Pb_{47}Tl_{53}$ and $Pb_{31}Tl_{69}$. Layers containing these mixtures as well as the pure materials were prepared and studied.

The layers containing thallium required cooling to liquid-nitrogen temperature in order to observe LEED patterns due to the large fluctuations inherent in systems that are unstable against the formation of CDW driven distortions. By contrast, the pure-lead layer showed well defined patterns at room temperature. Figures 1(b), 1(d), 2(b), 2(d) and 2(f) show schematically the LEED patterns obtained from all five samples, which with the exception of pure lead were observed with the sample at a temperature of 77 K. The features shown are a combination of all those observed in a primary-beam energy range covering 35 eV to 200 eV.

The proposed structures corresponding to the observed LEED patterns from pure lead and pure thallium (figures 1(b) and 1(d)) have been described elsewhere [3, 5] and are shown in figures 1(a) and 1(c) respectively. The lead chains have atoms equally spaced with a commensurability along the chain of three lead atoms to four copper atoms. The chains have been drawn along the furrows between copper atoms in the (001) direction since this is the most plausible registry. There is an empty furrow between chains placing them 5.12 \AA apart and neighbouring chains are displaced in the (010) direction by two copper atoms given the $[\frac{2}{2} \frac{2}{2}]$ unit mesh. The overlayer forms domains of structure such as that in figure 1(a) and an equivalent perpendicular arrangement.

The pure thallium chains (figure 1(c)) that are again separated by a distance of two copper atoms have an average spacing corresponding to a registry along the chain of five thallium atoms to six copper atoms. At low temperatures, however, they undergo a lattice distortion consisting of a dimerization with the result that equivalent thallium



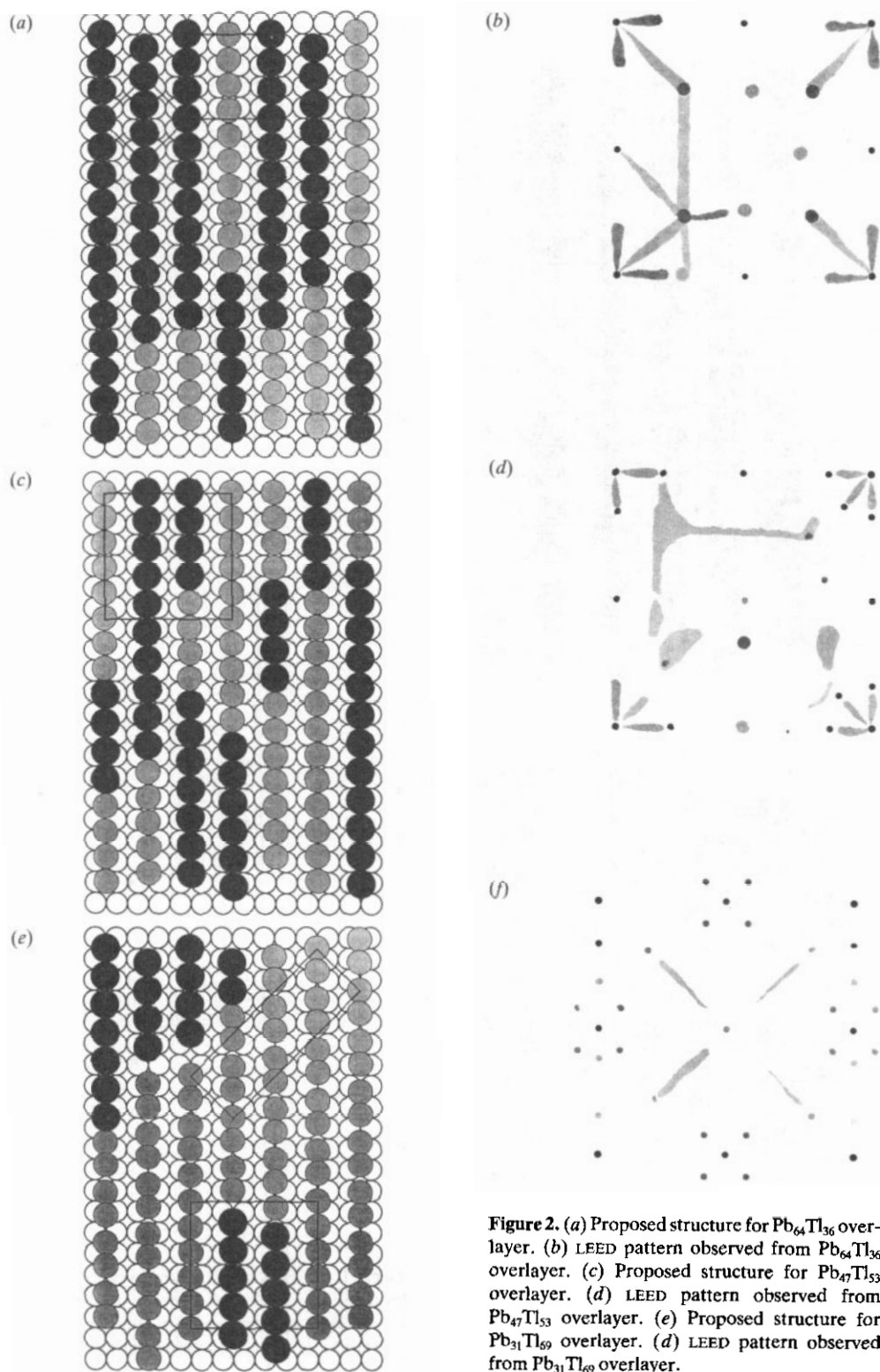


Figure 2. (a) Proposed structure for $\text{Pb}_{64}\text{Tl}_{36}$ overlayer. (b) LEED pattern observed from $\text{Pb}_{64}\text{Tl}_{36}$ overlayer. (c) Proposed structure for $\text{Pb}_{47}\text{Tl}_{53}$ overlayer. (d) LEED pattern observed from $\text{Pb}_{47}\text{Tl}_{53}$ overlayer. (e) Proposed structure for $\text{Pb}_{31}\text{Tl}_{69}$ overlayer. (f) LEED pattern observed from $\text{Pb}_{31}\text{Tl}_{69}$ overlayer.

atoms occur every twelve copper atoms. This produces a three-fold lengthening of one side of the $\begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix}$ unit mesh giving a $\begin{bmatrix} 6 & 6 \\ 2 & 2 \end{bmatrix}$ structure. It has already been suggested [5] that removal of the dimerization would result in a structure repeating every six copper atoms. Evidence for such a transformation is presented below.

The $\text{Pb}_{64}\text{Tl}_{36}$ overlayer LEED pattern (figure 2(b)) still contains all the $\begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix}$ spots indicating the existence of areas of the pure lead structure. The most significant change is the appearance of weak $\begin{bmatrix} 4 & 0 \\ 0 & 4 \end{bmatrix}$ spots. This structure would be produced by the removal of alternate chains in figure 1(a) and in this case is presumably due to the interpenetration of a thallium chain with a different structure. The atomic scattering factors of lead and thallium are almost identical, so the inequivalence of lead and thallium chains is due to their different atomic spacings. The $\frac{1}{4}$ -order streaks in the pattern are consistent with this intervening chain model where the registry between lead chains has been lost giving order, due to the repeat distance of four copper atoms along the chain, in 1D only. What is remarkable about the appearance of $\begin{bmatrix} 4 & 0 \\ 0 & 4 \end{bmatrix}$ spots is that it implies there are areas where parallel lead chains remain in registry over a distance of 10.24 Å despite the existence of an intervening thallium chain, though it is possible that the thallium chain is mediating the interaction. The proposed structure corresponding to figure 2(b) is shown schematically in figure 2(a).

Introducing more thallium into the overlayer to produce a $\text{Pb}_{47}\text{Tl}_{53}$ mixture results in the LEED pattern in figure 2(d). The brightest spots are those due to the substrate and the $(\frac{1}{2}, 0)$ spots common to the pure structures of both elements. Some $\frac{1}{4}$ -order streaking is also evident due to the intervening chains. The scarcity of features from either of the pure layers indicates a thorough intermixing of chains as shown in figure 2(c). The most notable new feature is the appearance of $\begin{bmatrix} 6 & 0 \\ 0 & 6 \end{bmatrix}$ spots. These would be produced by a repeat distance along the Tl chains of six copper atoms and their observation is compelling evidence for the existence of areas containing thallium chains that have the same density as the pure thallium structure but in which the Peierls distortion has been suppressed as postulated earlier. This could be the result of stress along the chain due to the existence of the areas of lead structure or an intermixing of lead valence electrons with the thallium valence band. This interpretation also requires commensurate alignment between Tl chains despite intervening Pb chains.

The pattern from the Tl rich $\text{Pb}_{31}\text{Tl}_{69}$ structure is shown in figure 2(f). This is predominantly the pure Tl pattern though the continued existence of some $\begin{bmatrix} 6 & 0 \\ 0 & 6 \end{bmatrix}$ spots indicates areas of undistorted Tl chains. The faint streaking reveals the existence of some Tl chains with an intervening Pb chain though this is far less evident than for the lead rich structure indicating a greater propensity for the formation of separate areas of the pure materials. The $\begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix}$ spots from the regions of pure Pb coincide with spots in the $\begin{bmatrix} 6 & 6 \\ 2 & 2 \end{bmatrix}$ pattern and so are not separately observable. Figure 2(e) shows a representation of the structures proposed.

In summary, we have shown that mixed Pb and Tl overlayers form interpenetrating chains with interaction between chains of one material despite intervening chains of the other. In the $\text{Pb}_{47}\text{Tl}_{53}$ and $\text{Pb}_{31}\text{Tl}_{69}$ overlayers there is evidence for the formation of Tl chains in which the Peierls distortion observed in the pure Tl overlayer has been suppressed.

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