Comment on "Computer Simulation of Coaxial Impact-Collision Ion Scattering Spectroscopy Spectra of Clean Pt(111) Surface and Pt(111)–p(2×2)-O Surface" [Jpn. J. Appl. Phys. 47 (2008) 7285]

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In a recent paper published by Takeuchi,[1] the atomic collisions in a crystalline target (ACOCT) simulation code was used to reanalyse co-axial impact collision ion scattering spectroscopy (CAICISS) data previously published in ref. 2. However, as the authors of the original article, we feel it is important to comment on several issues in Takeuchi's article.[1]

Firstly we draw attention to the correction factors used to adjust the screening length in the ion-atom interaction potential. The work of O'Connor[3] and ourselves[4,5] has clearly demonstrated that the correction factor is dependent on the atomic mass of the target atom. However, in Takeuchi's paper the He^+–Pt and He^+–O interactions have been assigned correction factors of 0.72 and 0.78 respectively. This clearly goes against the theoretical predictions for the variation of the correction factor with target atom mass which have been verified experimentally. Such errors result in erroneous shadow cone radii in the simulations and hence incorrect peak positions in the resulting angular spectra. Hence it is possible to obtain a reasonable fit of the experimental data using a combination of incorrect correction factors and trial structures.

The clean surface Pt(111) analysis presented by Takeuchi shows discrepancies of up to 5° between the peak positions in the experimental data and the ACOCT simulation results (particularly peaks III, IV, and V in Fig. 1[1]). This is most likely due to bulk Pt(111) being erroneously used as the trial structure. Previous work by Feder *et al.*[6] has shown outward relaxations in the region of 2% between the surface layer and the second layer, whilst we have determined the relaxation between the second and third layers to be around 6%.[5] As shown in Fig. 6 of Parkinson *et al.*,[2] discrepancies in these spacings are most likely to reveal themselves in two regions in the polar angle spectra, namely 30–70° and 100–150°.[2] Indeed, consideration of Fig. 6 in Parkinson's paper[2] and Fig. 3 in Takeuchi's paper[1] raises more doubts due to several second and third layer scattering geometries not being indicated in the latter case.

Fundamental problems also exist in the ACOCT analysis of the Pt(111)–p(2×2)-O surface. In our original work,[2] we clearly demonstrated one of the limitations which existed with our experimental setup at the time. Several minutes were required to acquire each spectra in the polar angle range, resulting in significant ion-stimulated desorption of the weakly bound O atoms from the Pt surface. As a result the data obtained from the Pt(111)–p(2×2)-O surface converged on to the clean Pt(111) spectra after a scattering angle of approximately 70° had been reached. Furthermore,

following the acquisition of the CAICISS data, X-ray photoelectron spectroscopy (XPS) revealed that most of the oxygen had been desorbed from the surface. Therefore Takeuchi's attempt to analyse the Pt(111)–p(2×2)-O surface using the full 180° experimental polar angle spectra cannot possibly yield the correct structure as the data begins with particles scattered from an oxygen-covered surface and ends with particles being scattered from a clean surface. Indeed, we clearly demonstrated the effects of ion-stimulated desorption and only the low-angle peaks could be used to glean information on the adsorption site of the O atoms. Whilst our results cannot be considered definitive they do not consider any data collected beyond a polar angle of 50° and thus the effects of ion-stimulated desorption in the analysis are significantly reduced.

We also urge caution in the comparison made with the work of Materer *et al.*,[7] whose Pt(111)–p(2×2)-O surface was prepared by adsorbing molecular oxygen (O_2) at room temperature, whilst our surface was prepared by saturating the surface using the more reactive atomic oxygen (O*) and annealing to 500 °C. As we previously described,[2] the different preparation methods would be expected to yield different locations for the O atoms in the near-surface region. We also note the use of the bulk Pt(111) structure in Takeuchi's analysis of the Pt(111)–p(2×2)-O surface which again leads to significant discrepancies between the experimental data and ACOCT simulations.

In conclusion we feel that the analysis of the clean Pt(111) and Pt(111)–p(2×2)-O surfaces using the ACOCT code presented by Takeuchi[1] must be treated with some uncertainty. It would appear that the author has used an incorrect screening length correction factor for oxygen and erroneously used the bulk Pt(111) atomic structure during the analysis of the CAICISS spectra. The analysis fails to appreciate the effects of ion-stimulated desorption during data acquisition and the likely differences in the location of O atoms resulting from different methods of preparing the Pt(111)–p(2×2)-O surface.

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