



Erratum

Erratum to: "Strong relaxations at the $\text{Cr}_2\text{O}_3(0001)$ surface as determined via low-energy electron diffraction and molecular dynamics simulations" [Surf. Sci. 372 (1997) L291]¹

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In the LEED intensity analysis, covered by the Erlangen group, the Debye temperature of oxygen was erroneously chosen to be far too low. The fit of all layer Debye temperatures to the experimental data, which has now been carried out in addition and in parallel to the structural parameters, changes the interlayer relaxation values. This is in contrast to general experience, according to which the consideration of thermal vibrations leaves the structure more or less unchanged but improves the quality of the theory–experiment fit. The latter is also true in the present case with the best-fit Pendry *R*-factor decreasing from 0.32 to 0.26.

Using the same procedure of analysis as in the original paper, the best fit develops for $\Theta_{\text{O}}=600$ K, $\Theta_{\text{Cr}}=630$ K and the interlayer distance relaxations (starting with the top layer) result in $a=-60\%$, $b=-3\%$, $c=-21\%$ and $d=+6\%$. In addition to the original work, the next interlayer distance between O- and Cr-layers was also varied and was found to relax by $e=+2\%$. The new values confirm our earlier message that the relax-

ations in $\text{Cr}_2\text{O}_3(0001)$ are strong. Again, we found the same lateral atomic arrangement as in the bulk. In particular, the new values determined for *a* and *b* are now in agreement with the results from the molecular dynamics simulations.

The new interlayer distances are mainly due to new positions of oxygen layers whilst the chromium sublattice remains more or less unmodified. So, for example, the sum of the two uppermost layer distances, separated by oxygen, remains practically unchanged. This strong correlation between *a* and *b* is due to the comparably weak scattering of oxygen which, generally, makes the determination of the oxygen layer positions less certain. Also, it indicates the need to consider cross correlations when error limits are calculated. This was not done in the original work – as is usual in LEED analyses – and so explains, why the error limits given earlier for the quantities *a*–*d* do not include the new parameter values. However, if one includes cross correlations in the error estimation, the errors amount to as much as 30–40% for the relative position of oxygen layers in the practically unchanged chromium sublattice. So, our earlier results lie within these more realistic and rather large error limits.

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