EPITAXIAL GROWTH OF THIN FILMS

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Received September 1, 1958

All the theories of epitaxial growth put forward so far either assume that a small misfit is an essential condition for the occurrence of an oriented overgrowth or they are based on the concept of basal plane pseudomorphism. According to Pashley the present experimental evidence does not completely support any of these assumptions. The degree of misfit, however, does appear to have some significance. In the light of this an attempt is made here to put forward a theory of oriented growth on oriented substrate. This theory is essentially an extension of the theory put forward (Dixit, 1933) for oriented growth on amorphous surfaces.

Metal atoms evaporated on cleavage planes of crystals

Dixit prepared thin films by evaporating metal atoms on flat amorphous surfaces. The electron diffraction study of these films showed fibrous orientations, which in their turn showed a characteristic dependence on the temperature of the substrate. This was explained by assuming that the atoms in such a layer behave like a two-dimensional gas and obey an equation \( \pi A = RT \),

where

\( \pi \) is the two-dimensional pressure (surface tension);
\( A \) is the area occupied by the atom on the substrate;
\( R \) is the gas constant

and

\( T \) is the absolute temperature.

The evaporation of metal atoms on the cleavage planes of crystals, however, introduces a significant difference in our considerations. An amorphous flat surface only serves as a reasonably flat support and there is no interaction between the atoms of the substrate and the deposited atoms. The cleavage surface not only serves as a flat support, but there will also be a force of attraction between the ions of the substrate and the deposited neutral metal atoms. (As before we shall consider the formation of the first atomic...
layer only.) The additional force of attraction, which now manifests itself between the ions of the substrate and the deposited neutral metal atoms, can be reasonably assumed to be of the polarisation or van der Waals' type. This force will introduce an additional term in the equation already given, which will depend on the van der Waals' energy and the area occupied by the atom. The equation thus becomes:

\[ \pi A + ACr^{-6} = RT \]

where \( r \) is the distance between the two atoms, one of the substrate and the other of the deposit.

or

\[ r^2 = r_1^2 + r_2^2 + l^2 \]

where

\( r_1 \) is the atomic distance for the substrate;
\( r_2 \) is the atomic distance for the deposit

and

\( l \) is the distance between the two planes, namely, the substrate plane and the deposit plane.

In the above equation if the term \( ACr^{-6} \) is absent we get the same relation as before, showing orientation as a function of the temperature. The effect of this term is to effectively reduce the term \( RT \) on the right-hand side, \( i.e., \) the temperature at which any particular \( \psi \) occurs in the presence of the attractive force of the substrate is less than the temperature at which the same orientation would occur in the absence of the attractive force, or the epitaxial temperature will be less than the amorphous orientation temperature. Further, even here as before

\[ A_{111} < A_{100} < A_{110} \]

and therefore

\[ T_{111} < T_{100} < T_{110}. \]

Both these conclusions appear to agree with experimental observations.\(^{1-9} \)

The modifying term can be written as:

\[ ACr^{-6} = AC \left( r_1^2 + r_2^2 + l^2 \right)^{-3} \]

\[ = ACr_1^{-6} \left\{ \left( \frac{r_2}{r_1} - r_1 \right) \left( \frac{r_2}{r_1} + 2 + \frac{l^2}{r_1^2} \right) + 2 + \frac{l^2}{r_1^2} \right\}^{-3} \]

\[ = ACr_1^{-6} \left\{ \text{misfit} (\text{misfit} + 2) + 2 + \frac{l^2}{r_1^2} \right\}^{-2} \]