Domain structure in oxygen on a Cu(110) surface

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A theory is derived for the domain structure in a system of adsorbed oxygen atoms on a Cu(110) surface.

A periodic stripe domain structure was recently observed[1] in a system of oxygen atoms adsorbed on a copper (110) surface (Fig. 1). Each domain is a macroscopic 2D uniform phase. One of these phases has a monatomic layer of oxygen in a (2×1) structure, and another has a gas of oxygen atoms. The possibility in principle that such domain structures would exist stems from the strictive instability which was established more than a decade ago.[2] Below we calculate the period of this stripe domain structure as a function of the concentration of the phases. The theory presented below is in satisfactory quantitative agreement with the observations of Ref. 1.

When a crystal is deformed, the surface energy changes by an amount

$$\int \beta_{\mu\nu} u_{\mu\nu} dS \tag{1}$$

in the approximation linear in the deformation. Here $\beta_{\mu\nu}$ is the surface-tension tensor, and μ and ν are the x and y components tangential with respect to the surface.[3] In each of the states which coexist in this domain structure, there are, in accordance with their symmetry, C_{2v}, two independent components: β_{1xx}, β_{1yy} and β_{2xx}, β_{2yy}. The jump which occurs in these components as the 2D phase boundary is crossed signifies the presence of a surface force which is acting on the interior of the crystal. The deformations which arise are favored from the energy standpoint, since the surface component

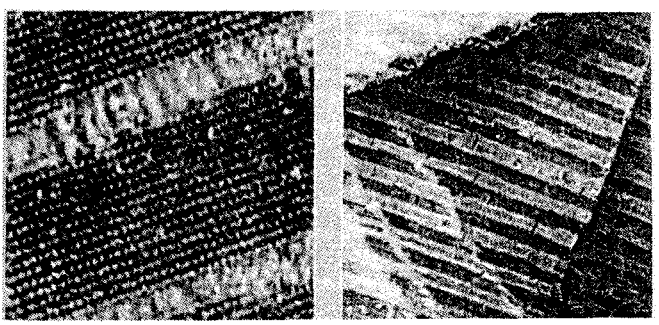

FIG. 1.

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of the energy is linear in the deformations. The magnitude of the advantage in terms of the energy, on the other hand, has a logarithmic divergence. This divergence is responsible for the appearance of this domain structure. The period of the structure, d, is found by minimizing the energy density of the structure:

$$\frac{\gamma}{d} - \frac{A}{d}(\beta_{1xx} - \beta_{2xx})^2 \ln \frac{d}{af}, \tag{2}$$

where γ is the usual energy of a line separating surface phases, a is a characteristic atomic spacing, $f = f(c)$ is an unknown function of the phase concentration c, and the constant A is a definite function of the elastic moduli of the crystal. In the isotropic case, for example, it is[2,4]

$$A = \frac{(1-\sigma^2)}{\pi E},$$

where E is the Young's modulus, and σ the Poisson ratio.

The function f was in fact calculated in Ref. 4 for an isotropic crystal. We can show that the result derived there also applies to the structure under consideration here, on a (110) surface of a cubic crystal. The strain field u_{xx} at the surface caused by the linear distribution of the surface force $F_x = \beta_{1xx} - \beta_{2xx}$ falls off in accordance with

$$u_{xx} = -AF_x x^{-1}, \tag{3}$$

where the constant A is the same at $x > 0$ and $x < 0$ by virtue of the symmetry. By virtue of the linearity of elastic theory, the strain reduces to the sum of the strains from all the boundaries between domains:

$$u_{xx} = AF_x \sum \left(\frac{1}{nd - x} - \frac{1}{nd + cd - x} \right). \tag{4}$$

The sum of the energies in (1) and of the bulk elastic energy for an equlibrium deformed state reduces to the surface integral [cf. Eqs. (1)–(2) in Ref. 4].

$$\frac{1}{2} \int \beta_{\mu\nu} u_{\mu\nu} dS. \tag{5}$$

Substituting expression (4) into this integral, integrating (here we introduce a cutoff parameter a to eliminate the logarithmic divergence at short distances), and summing the resulting series of logarithms, we find the following expression for the function $f(c)$:

$$f = c \prod_{n=1}^{\infty} \{1 - (c/n)^2\} = \frac{1}{\pi} \sin \pi c. \tag{6}$$

Minimizing the energy in (2) with respect to the period of the structure, we find

$$d = \frac{\Delta}{\sin \pi c}, \tag{7}$$

where the quantity Δ is an exponetial function of the characteristics of the surface

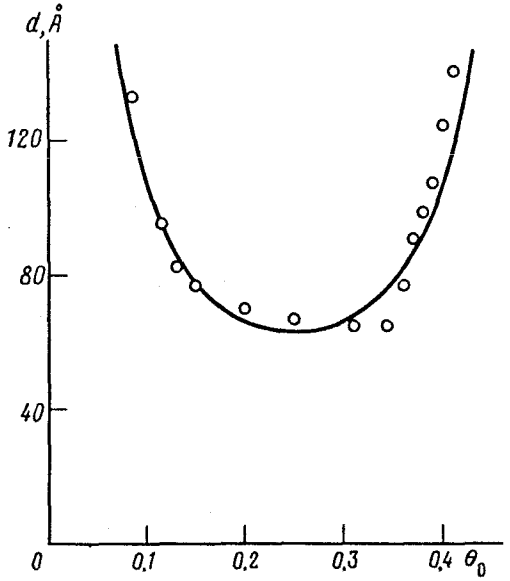

FIG. 2.

phases and of the elastic constants of the crystal. Consequently, the period of the structure may be macroscopic.[2]

If we ignore the density of oxygen atoms in the 1×1 phase, and if we furthermore ignore oxygen defects in the 2×1 structure, then we find that the concentration c is determined unambiguously by the parameter θ_0. This parameter is the fraction of vacancies in the first adsorption layer which are filled by oxygen atoms:

$$c = 2\theta_0. \tag{8}$$

The points in Fig. 2 show observational data of Ref. 1 on the period of the domain structure as a function of the oxygen filling at a temperature of 640 K. The curve shown here is theoretical, calculated from (7) with the help of (8). The parameter Δ was taken to be 63 Å.

It is not difficult to see that incorporating electrostatic effects, which would also make a negative logarithmic contribution of the boundary energy of the 2D phases at the surface (§3 in Ref. 4), would lead to only a renormalization of the parameter A in expression (2).

We also note that a 2D stripe domain structure which arises because of the logarithmic boundary energy is unstable in the isotropic case.[5] In the case discussed above, on the other hand, in which the energy of the line separating the 2D phases, γ, is a function of the orientation of this line on the surface, and there is an anisotropy in the elastic constants, the conditions for stability of the stripe structure could definitely be satisfied.

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