

Contributions Regarding the Influence of Crystallization System on Metals Deformability

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Abstract: To reconsider the computation method of the atomic density of the crystallographic plans and to propose that when computing it the number of atoms to be replaced with the surface covered by the atoms.

On the basis of the computation method proposed by the authors, the maximum atomic density plans (gliding plans in the case of plastic deformation) belong to the cubical crystalline network with centered volume and not cubical with centered surface. In consequence, the maximum deformation will be mastered by the metals, which crystallize in the cubic system with centered volume.

In order to support this recommendation it has to be presented also some examples of interdependence between the atomic density of the crystallographic plans and metals deformability.

Among the factors that influence metal's deformability, (examples: the nature and density of network flaws, purity etc.) there is also the crystallization system, including the nature of the crystalline network.

In spite of numerous studies and research regarding the influence of the crystallization system and of the crystalline network on metal deformability, especially on the plasticity, the interdependence between the crystallization system and deformability it is not well known. Although it has been established that during plastic deformation atoms sliding takes place preferentially, and some times exclusively, along the crystallographic plans of maximum atomic density, called also sliding plans, the nominalization of these plans is not fully established.

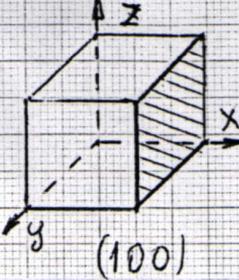
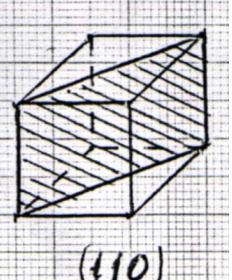
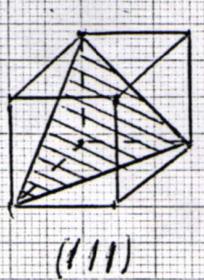
Initially it has been considered that the atomic density of a crystallographic plan can be expressed through the number of atoms that belong to the analysed plan. On this basis, the following conclusion arose: the maximum atomic density plans belong to the cubic crystalline network with centered surfaces and in consequence, the metals that are easier to be plastically deformed are the ones that crystallize in the cubic system with centered surfaces. This conclusion has been assimilated by the majority of researchers in the field of physical metallurgy and that of metal material processing through plastic deformation, and it can be found in all the specialty works of the two interest areas [2], [3], [4], [5], [6], etc.

In table 1 there are presented the values for atomic density for the main crystallographic plans from the cubic system, cubic networks with centered volume (*cvc*) and cubic with centered surfaces (*cfc*) calculated in the above hypothesis, meaning that the atomic density of a crystallographic plan is equal to the number of atoms that belong to the analysed plan.

From the analyse of the atomic density values presented in table 1, on first sight, results that the crystallographic plans with the highest atomic density belong to the cubic network with centered surfaces. Based on these values, the conclusion that maximum plasticity is

possessed by the metals that crystallize in the cubic system with centered surfaces. On a closer look it can be observed that these values are not real, because when computing them it was not taken into account the surface of the crystallographic plan and that occupied by the atoms. From the graphs included in table 1 it can be easily observed that the plan's surface (100) is smaller than the plan (110) but bigger than that of the plan (111). Also, it has to be taken into account that a marginal atom, as the atoms from the corners of the crystallographic plan, occupies a surface smaller than that of a central atom, situated at the intersection of diagonals.

Table 1.

| Plan's Orientation and Miller indexes |  <p>(100)</p> |  <p>(110)</p> |  <p>(111)</p> |
|---------------------------------------|--|--|---|
| Crystalline Network | Atomic density | | |
| Cubic simple | 0,5 | 0,5 | 0,375 |
| Cubic with centered volume | 0,5 | 1,0 | 0,875 |
| Cubic with centered surfaces | 1,0 | 1,5 | 1,875 |

In order to correct these inadvertences it is necessary that the atomic density of the crystallographic plans to be calculated on the basis of the relation between the occupied surface of the atoms intersected by the crystallographic plan and the plan's surface and not on the basis of atoms number that belong to the analysed plan.

In table 2 it is centrally presented, for the main plans of the cubic crystalline network with centered and cubic volume and centered surface, plan's surface, number of atoms on a plan, atom's surface, the surface occupied by the atoms on a plan and the atomic density.

In this case in order to compute the surface of the plans and atoms it was used as measure the surface of a face of the elementary cell and the atomic density was established on the relation between the surface occupied by the atoms and the surface of the crystallographic plan.

From table 2 it can be observed that the plans with higher density belong to the cubic crystalline network with centered volume and not to the one with centered surface. The atomic density is of 100% for the plans belonging to the (111) family, of the cvc network, can be explained by the modifications to the configuration of the atoms belonging to these plans. In this case the atoms configuration, or at least that of the central atom is no longer spherical and resembles to elastic spheres which due to lack of space in the recipient in which they were put have deformed and occupied the free spaces. With regard to the volume of the free spaces from the elementary cell of the cvc system it is to be mentioned that this cell has atomic compact ability of 68%, which means that these spaces represent 1/3 of the cell's volume.

Table 2.

| Crystallographic Plan | | (100) | (110) | (111) |
|-------------------------------|-----|-------|-------|-------|
| Plan's Surface | | 1,0 | 1,41 | 0,87 |
| Number of atoms | cvc | 1,0 | 2,0 | 1,5 |
| | cfc | 2,0 | 2,0 | 2,0 |
| Atom's surface | cvc | 0,585 | 0,585 | 0,585 |
| | cfc | 0,391 | 0,391 | 0,391 |
| Surface occupied by the atoms | cvc | 0,585 | 1,17 | 0,87 |
| | cfc | 0,782 | 0,782 | 0,782 |
| Atomic density, % | cvc | 58 | 82 | 100 |
| | cfc | 78 | 55 | 89 |

Taking into account the atomic density of the two crystalline networks it results that the metals with the best deformability are the ones that crystallize in the cubic system with centered volume and not cubical with centered surfaces, as considered until now.

The fact that metal's plasticity, as component of deformability, is higher in the case of cubic crystalline network with centered volume than in the case of cubic network with centered surfaces results also from figure 1.

In figure 1 it is presented the variation of plasticity in relation with temperature, for the iron with industrial purity in the two allotropic state, meaning the α state with the cubic crystallization with centered volume and γ state with cubic crystallization network with centered surfaces [1].

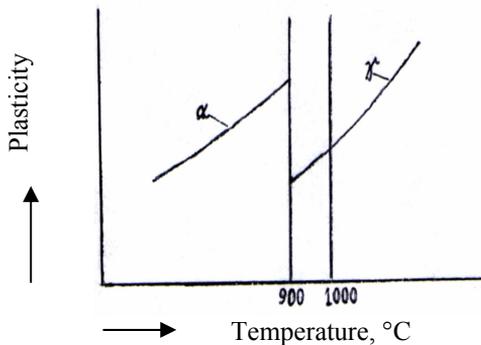


Fig. 1. The influence of temperature on the α and γ plasticity.

From figure 1 and table 2 it results that the plasticity is higher in the case of cubic crystalline network with centered volume.

In figure 2 it is presented the resistance variation at plastic deformation, in relation with temperature, for plain carbon steel and with low carbon content.

In figure 2 it can be observed that after the state transformations $\alpha \rightarrow \gamma$, in the temperature interval 700-800°C, in the austenite area, with the crystallization system cfc, the resistance at plastic deformation is higher than in the ferrite - pearlite domain, the domain where it prevails ferrite with cubic crystalline network with centered volume.

Because metal's deformability is directly proportional with plasticity and inverse proportional with the resistance for plastic deformation from figures 1 and 2, results, that between the two crystalline networks of the cubic system, that the cubic network with centered volume has the maximum deformability.

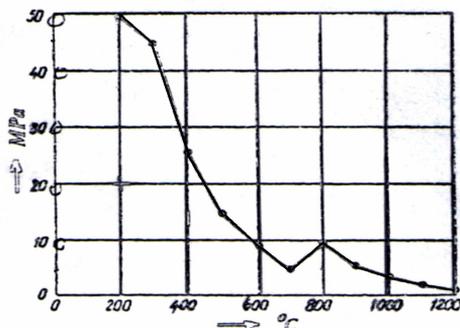


Fig. 2. The influence of temperature on the resistance to plastic deformation on plain carbon steel

In comparison with metal's deformability that crystallizes in the cubical system, indifferent of the crystalline network, metal's deformability, which crystallizes in the hexagonal system, is reduced. The reason for the diminish in metal's deformability, especially of the plasticity, which crystallize in the compact hexagonal system, as presented in the specialty literature [2, 4], etc, is constituted by the reduced number of sliding plans. Metals that crystallize in the compact hexagonal system have only one sliding plan, base plane.

As a general conclusion, it can be said that the framework of the two crystallization systems, cubic and hexagonal, systems that crystallize the majority of metals (over 50 metals), from the point of view of deformability, on the first place can be found the cubic system with cubic crystalline network with centered volume, and on the last place the compact hexagonal system. The cubic system with cubic network with centered faces is situated on the second place and not on the first place as considered until now.

References:

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