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"Intergranular Friction Based Model For Yield Strength Of Nanocrystalline Materials"

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Most of models have been proposed to explain dependence of yield strength on grain size in nanocrystalline materials. They have explained this only by extrapolating classical Hall-Petch equation [20, 21]. Also many of the models have certain limitations.

An intergranular friction based model is proposed to explain the dependence of yield strength on grain size of nanocrystalline materials. In this model, we have considered that intergranular friction at the grain boundaries in nanocrystalline materials. The intergranular fiction based model shows good agreement with corresponding experimental data.

Keywords: Friction; Hall – Petch; Inverse Hall-Petch; Yield strength; nanocrystalline materials

Introduction

Nanocrystalline materials are the polycrystalline materials having grain size in nanometre (1 to 100 nm) range. Nanocrystalline materials have several applications in wide range of fields because of their improved physical, mechanical and chemical properties as compared to course grained materials [3].

For polycrystalline materials, it is well known that as the grain size of the crystal decreases, the yield strength of the polycrystalline material increases based on classical Hall-Petch equation [1, 2]

which can be expressed as

$$\sigma_y = \sigma_0 + k\, d^{-1/2} \qquad (1)$$

Where d is the average grain diameter, σ_y is the yield strength, σ_0 is the friction stress below which dislocation can not move in the crystal and k is a constant called 'locking parameter' representing the relative hardening contribution of the grain boundary.

Experimental data available in literature [4, 8, 18] for the Nanocrystalline materials shows that the yield strength of Nanocrystalline material can no longer be described by classical Hall-Petch equation and hence Hall-Petch equation is not useful as far as Nanocrystalline materials are concerned.

At present there are many theoretical models explaining abnormal Hall-Petch effect and Inverse Hall-Petch effect in Nanocrystalline materials and claiming agreement with corresponding experimental data. Most of the models proposed to explain the Hall-Petch behaviour in nanocrystalline materials are based on following deformation mechanism

1) Grain boundary sliding 2) Grain boundary diffusional creep [8] and 3) Dislocation [6, 7].

The models explaining Inverse Hall-Petch effect includes 1) Dislocation based models [9, 13] 2) Diffusion based models [14, 15] 3) Grain boundary shearing models [18] and 4) Two phase based models [5].

Many of the above mentioned models have certain limitations. In Malygin's model [7], the stress calculated is not a yield stress. Also the dislocation based models are unable to explain the dependence yield stress at sufficiently small grain size and hence unable to explain abnormal Hall-Petch effect in Nanocrystalline materials properly. Also there are many models which explain only either Hall-Petch or Inverse Hall-Petch effect. Though the researchers trying to explain the phenomenon by proposing various models but the problem is yet unsolved and controversy still persist. Also because the Nanocrystalline materials shows complete deviation from classical Hall-Petch relation, then simply extrapolation of the classical Hall-Petch equation can not be the solution to the problem.

In the present paper we have proposed a model based on the new idea of intergranular friction which has no relation with classical assumption of dislocation based grain boundary deformation which forms the basis for Hall-Petch relation in coursed grained materials.

Description of model:

In the intergranular friction based model, we have assumed that grain posses very high surface roughness at grain boundaries. We know that the secret of inherent properties of nanocrystalline materials that differs it from bulk material lies in considerable increase in surface area to volume ratio. Again, for nanocrystalline materials, as grain size decreases there is considerable increase in number of grains per unit volume and hence the considerable increase in volume fraction of grain boundaries. Considering all this factors we can say that frictional force at grain boundaries per unit volume for nanocrystalline material must have to increase. Therefore more external force is required to deform the system and hence yield strength increases with decrease in grain size.

By considering intergranular friction at grain boundaries for nanocrystalline material of unit volume, we have derived relation for yield strength of nanocrystalline material as below.

Let 'F' be the total frictional force at grain boundaries inside nanocrystalline material of unit volume. Hence F is given by

$$F = \mu\ g\ \frac{m(\text{no.of grains})}{\text{volume}} \times (\text{surface area})\ \frac{\text{no.of grains}}{\text{volume}} \qquad (1)$$

$$F = \mu \left(\rho\ \frac{4}{3}\pi\ r^3\right) \times \left(\frac{1}{\frac{4}{3}\pi\ r^3}\right) \times 4\pi r^2 \times \left(\frac{1}{\frac{4}{3}\pi\ r^3}\right) \qquad (2)$$

Where, m is mass of each grain.

g is acceleration due to gravity

μ is coefficient of friction

ρ is relative density of material and

r is grain radius.

Therefore, $F = \frac{3\mu\rho g}{r}$ (3)

But, Yield stress = $\sigma = \frac{F}{A}$ (4)

Therefore, $\sigma = \frac{3\mu\rho g}{r\ A}$ (5)

Also we have assumed that the actual surface area of grain in contact with the surrounding grains is less than that of the surface area of grain. We have defined a factor which gives the fraction of actual surface area of grain in contact with the surrounding grains to the surface area of grain and we called it as 'occupancy factor'. Therefore equation (5) is modified as

$$\sigma = k\frac{3\mu\rho g}{rA} * P \qquad (6)$$

Where, 'P' is occupancy factor which is found to be function of 'r' as

$$P = f(r) = e^{-\frac{r_0}{r}} \qquad (7)$$

In equation (6), K is material dependent constant and r_0 is critical grain radius.

and μ is coefficient of friction which is found to the function of grain size d as

$$\mu = e^{-\frac{0.2\ x}{d}} \qquad (8)$$

In equation (3), x is height of surface roughness and is given by

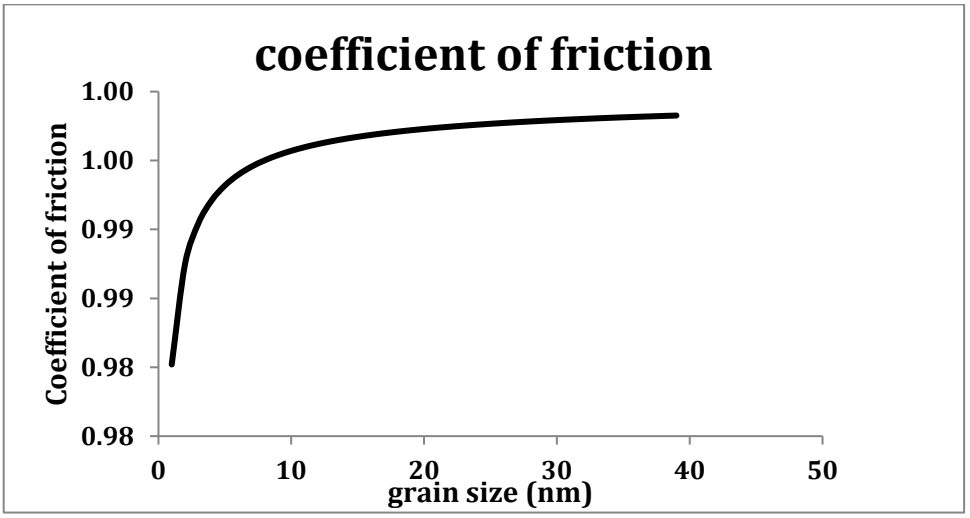
$$x = \frac{d^{1/3}}{10} \qquad (9)$$

Equation (1) can be rewrite as,

Yield strength $\sigma = \frac{3\mu\rho g}{rA}\, k\, e^{-\frac{r_0}{r}}$ (10)

Results and Discussion

From equation (8) it is clear that, in nanocrystalline materials the coefficient of friction μ is not a material dependent but a function of grain size'd' only. The variation of coefficient of friction with grain size is as shown in fig. (1).



From equation (7) it is clear that, what differ nanocrystalline materials from each other is occupancy factor P as is depends on critical grain radius $r_0$which are material dependent. The variation of occupancy factor p with gain size d for Fe and Cu is as shown in fig (2) and fig (3) respectively.

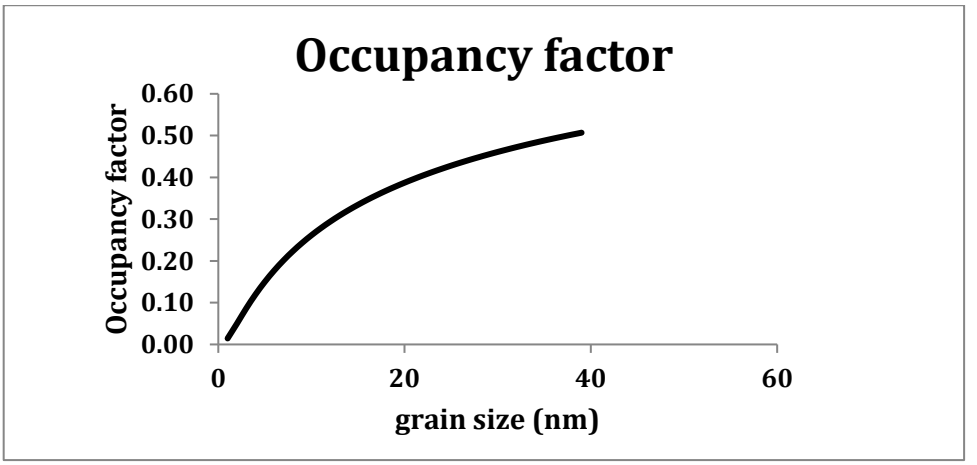


Fig (2): Variation of occupancy factor p with gain size d for Fe.

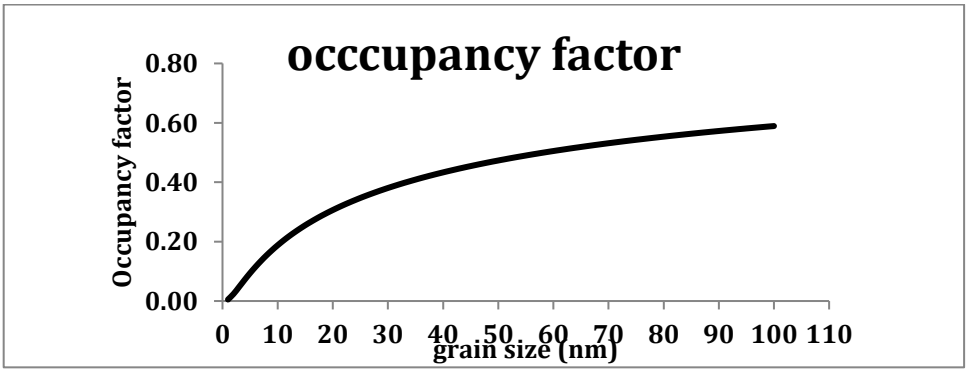


Fig (3): Variation of occupancy factor P with gain size d for Cu.

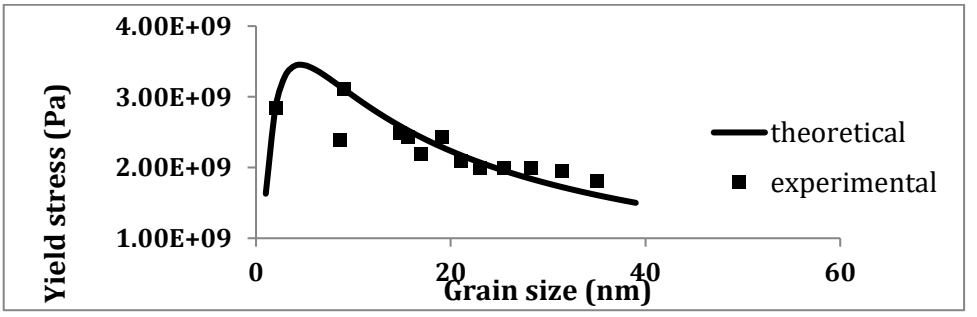


Fig (4): Comparison of theoretical prediction of the model from equation (10) with experimental data [13] for Fe.

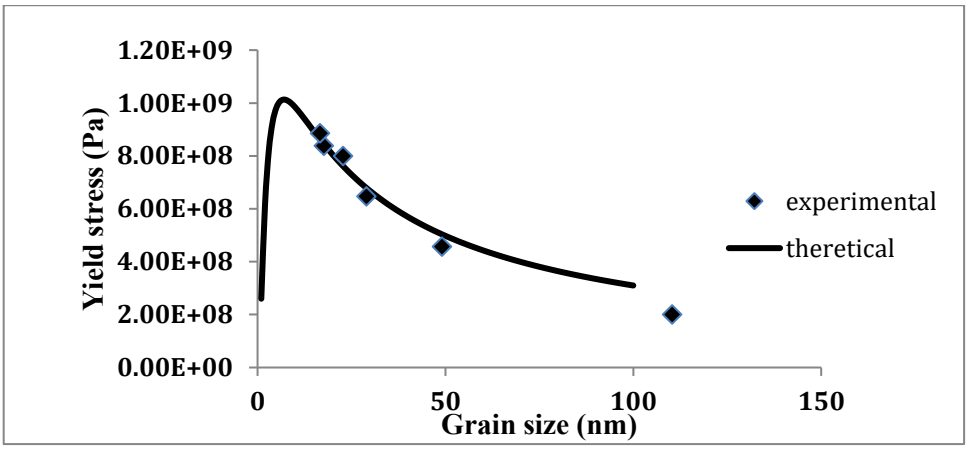


Fig (5): Comparison of theoretical prediction of the model from equation (10) with experimental data [22] for Cu.

From Figure 4 and 5, it is clear that results obtained from model shows good agreement with the corresponding experimental data. It holds good in both abnormal Hall-Petch and Inverse Hall-Petch region.

Conclusions

The model herein assumes intergranular friction at grain boundaries in nanocrystalline materials. Model shows good agreement with the experimental data. It holds good in both abnormal Hall-Petch and Inverse Hall-Petch region**.** So it is conclude that the intergranular friction is behind the abnormal Hall-Petch behaviour in Nanocrystalline materials.

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