

## Enhancing nanocrystalline material yield strength during ARB process by using Solute atoms as reinforcement

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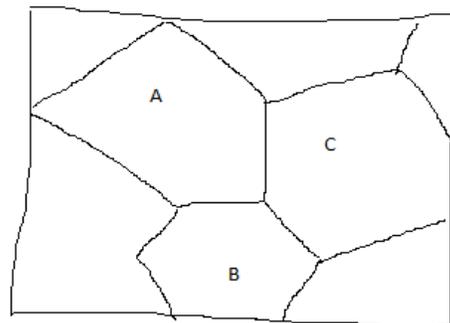
**Abstract**—In the current study solute atoms are used as reinforcement during ARB process. During the process of ARB dislocation line entanglement usually occurs in the grains, causing the formation of a jog which opposes dislocation motion during material deformation. These entanglements and jogs act as pinning points in the material during ARB process. The mobility of materials dislocation are more complex when the material are being deformed at elevated temperature as grain growth also takes place that negatively impacts the yield stress. To prevent grain migration and dislocation and even transfer of heat from one grain to other solute atoms are used as reinforcement during ARB process. Little studies have been done on thermal stability by studying the pinning points in the material and enhancing the material property to be more stable with high control dislocation process during grain refinement. In the current study focus is giving in material stability during grain refinement at elevated temperature by studying the dislocation of grain boundaries mobility. The following facts are revealed in modeling. It was shown that the yield stress increase to an ultimate yield stress which was accompanied by decrease in yield stress as hardness during particle cutting and hardness for particle bowing decreases. It was also shown that the change in yield stress and shear stress increase with time during ARB process. It was shown that the creation of second phase might also be created by mechanical or thermal treatments process during ARB. It is observed that the particles that compose the second phase cause pinning points.

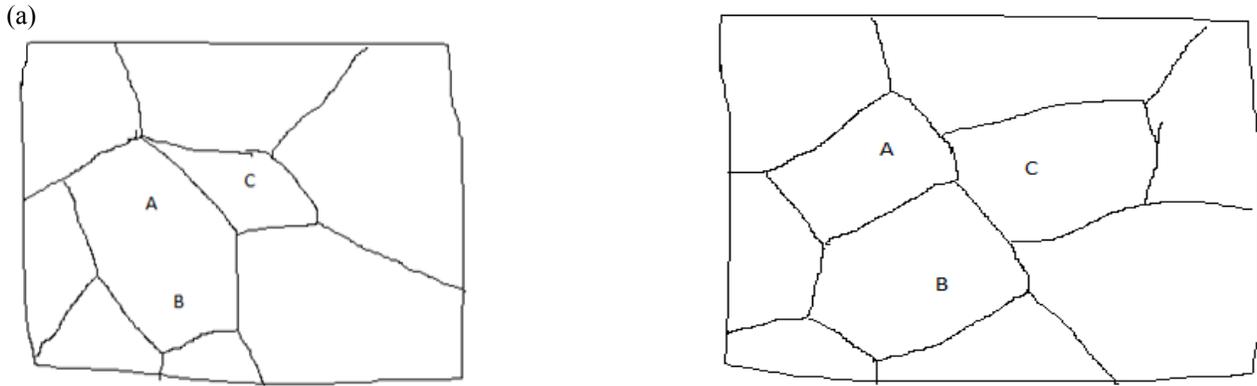
**Keywords:** Yield stress, hardness, ARB, temperature and size

### Introduction

Severe plastic deformation induced grain growth has been widely reported in various plastic deformation techniques including nano-indentation, high pressure torsion, uniaxial tension and uniaxial compression [1-5]. The grain growth

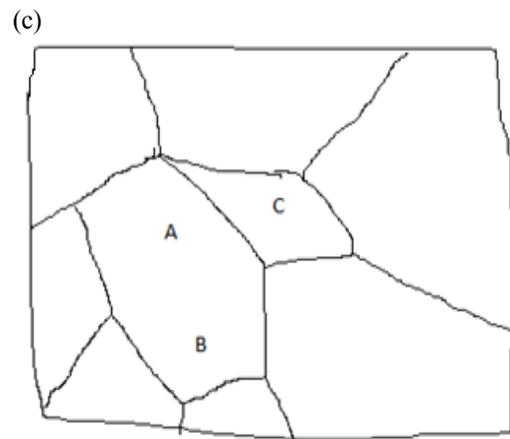
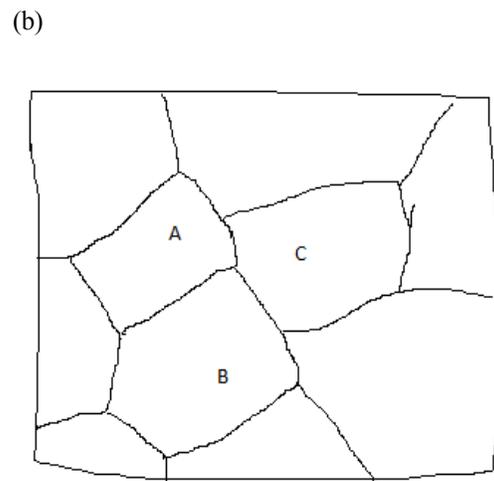
changes the structures of nanocrystalline materials and therefore affects their mechanical properties [1-7]. Molecular dynamics simulations and theoretical analysis have been carried out to understand the mechanisms of deformation inducing grain growth, and contradictory results have been reported [1-9]. Grain rotation and coalescence process takes place when grains rotate and join as a single grain. It brings about a change in the size of a grain at any instant when the misorientation angle between some adjacent grains becomes zero [8-13]. The time evolution process shows grain rotation of grain A towards grain B and coalescence with grain B resulting in elongated grain A-B as shown in Figure 1 (a-b) [9]. In the initial configuration the two grains are disoriented by approximately 180° [9]. During the initial deformation grain A, B and C shrink due to GB migration, while grain B has already undergone some significant rotation towards the orientation of grain A [9]. It is further observed that grain B, has actually grown again due to continuous rotation [9]. It is also important to know that the inclination of GB migration between grains A and B has changed during this process. Finally the coalescence of grains A and B is observed in Figure 1(b) where two grains now being closely aligned with low-angle GB between them was reduced to single dislocation [9].





(b)  
 Figure.1. Grain Rotation Processes (Haslam et al. 2001:22).

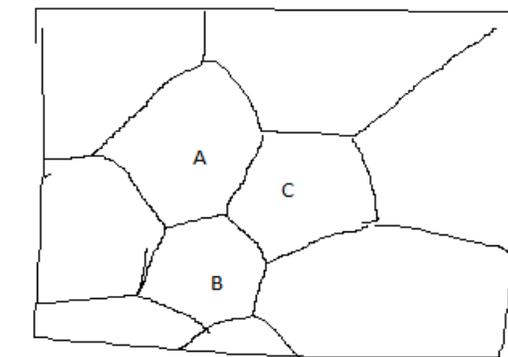
Figure 2 (a) is a complementary view of grain rotation-coalescence mechanism [9]. The diagram in Figure 1 (b) revealed that rotation-coalescence may be seen as “unzipping” of the GB between the two grains with larger angle approximately 180 and high concentration of miscoordination in the GB between grain A and B [9]. Figure 1 (a-b) showing a very high concentration of miscoordination in the GB between grains A and B after a very short period. It is observed in Figure 2 (a) that the misorientation angle has reduced to approximately 16.50 with the creation of a dislocation structure of the GB. Three well separated GB dislocations can be observed in Figure 2 (a) and after a short period of time the misorientation angle decreased to about 90 and the dislocations left are shown in Figure 2 (b). The change in inclination of the GB between grains A and B observed in Figure 2 (c) and Figure 2 (d) coincides with this absorption. With the low remaining misorientation angle of about 40 after a short period of time as shown in Figure 2 (d) only the dislocation at the centre of the GB remains.



(d)

Figure.2. Grain Rotation Processes and Coalescence [9].

The force law governing GB migration and GR is given by Newton’s law of motion coupling the acceleration of the atoms to the force acting on them [9]. A constant driving force for migration,  $P$  results in a constant drift velocity



(a)

given by  $V = mp$  [9] where  $m$  is the GB mobility, which is a parameter such as the GB energy and it depends on the GB misorientation and the crystallographic orientation of the GB plane [9]. From the viscous force law  $V = mp$  the mobility is independent of both the driving force and the mechanism of GB migration (Haslam et al., 2001:22). Since the applied force is at an angle, the mobility can be expressed with a force law which is similar to angular velocity of a rotating grain,  $\omega$  with respect to an axis through its centre of mass  $\omega = M\tau$  (Haslam et al., 2001:22) where  $M$  is the rotational mobility of the grain subjected to a torque  $\tau$ .

It is reported that some grains experience a net torque for rotation, provided that the total GB energy across all the surface of the neighbouring grains decreases as a result of the rotation (Haslam et al., 2001:22). The rotational mobility of a non-spherical grain embedded in a more or less rigid matrix of all the surrounding grains is strongly influenced by its shape (Haslam et al., 2001:22). The rotation of such a grain necessitates a continuous accommodation process (Haslam et al., 2001:22). Two accommodation mechanisms based on GB diffusion or dislocation motion exist (Haslam et al., 2001:22). At high temperatures the diffusion-accommodation process is more acceptable assuming a hexagonal grain shape within a columnar microstructure and diffusion acts as the accommodation mechanism (Haslam et al., 2001:22). It must be noted that Plastic deformation usually occurs when large numbers of dislocations move and multiply during grain refinement process [1-7]. To enhance the mechanical property in a material (i.e. increase the yield and tensile strength), it is vital to introduce a mechanism which prohibits the mobility of these dislocations during grain refinement. This mechanism may be, (work hardening, grain size reduction, etc.) since they hinder dislocation motion and render the material yield stress and tensile strength stronger [1-6]. The stress required to cause dislocation motion is orders of magnitude lower than the theoretical stress required to shift an entire plane of atoms, so this mode of stress relief is energetically favorable during grain refinement process. Therefore material yield and tensile strength greatly depend on the ease with which dislocations mobility during grain refinement. Normally the pinning points, or locations in the crystal that oppose the motion of dislocations during grain refinement can be introduced into the lattice to reduce dislocation mobility, thereby increasing mechanical strength of the material

during grain refinement [5]. Material dislocations process may be pinned due to stress field interactions in the material during deformation process with other dislocations and solute particles, creating physical barriers from second phase precipitates forming along grain boundaries during grain refinement process. Usually there are five main strengthening mechanisms for metals. Each of this strengthening mechanism prevents dislocation motion and propagation, or makes it energetically unfavorable for the dislocation to move during grain refinement process. For a material that has been strengthened, by some processing method, the amount of force required to start plastic deformation is greater than it was for the original material.

Material strengthening is mainly caused by grain dislocations process. Dislocations interact with each other and create fields in the material during deformation. The interaction between the stress fields of dislocations during grain refinement might impede dislocation motion by repulsive or attractive interactions during deformation. During grain refinement process, if two dislocations cross during refinement, dislocation line entanglement usually occurs in the grains, causing the formation of a jog which opposes dislocation motion during material deformation. These entanglements and jogs act as pinning points in the material and this oppose dislocation motion. As both of these processes are more likely to occur when more dislocations are present, there is a correlation between dislocation density and yield strength. The mobility of materials dislocation is more complex when the material is being deformed at elevated temperature as grain growth also takes place that negatively impacts the yield stress and tensile strength of the material. Thermal stability in nanomaterials is a hot spot area in materials study due to the complexity of grain growth. Little studies have been done on thermal stability by studying the pinning points in the material and enhancing the material to be more stable with high control dislocation process during grain refinement. In the current study focus is giving in material stability during grain refinement at elevated temperature by studying the dislocation of grain boundaries mobility.

### Methodology

Material hardenings are mainly caused by dislocations during grain refinement. The dislocations interact with each other and generate field stresses in the material during grain refinement. The field stress interaction caused by dislocation impedes dislocation motion due to their repulsive or attractive interactions during grain refinement.







