

# A new statistical mechanics approach to model deformation in metals



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Fundamentals of Advanced Materials

## Basic concepts

The plastic deformation of metals is mostly carried out by lattice defects such as dislocations, vacancies and grain boundaries. Dislocations play a key role in such process.

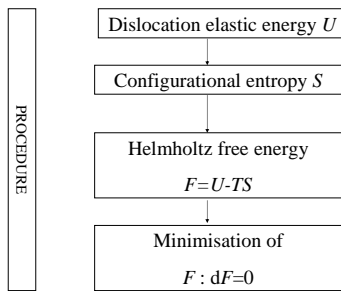
Deformation parameters such as:

**flow stress, strain and strain rate**

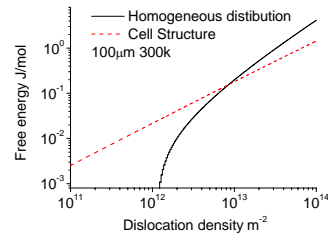
depend on

**dislocation density, grain size, recovery and recrystallization.**

Our challenge is to relate these factors by employing STATISTICAL MECHANICS.



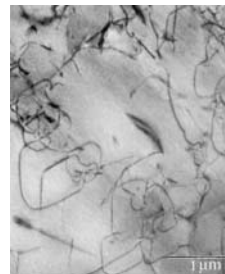
## Typical results



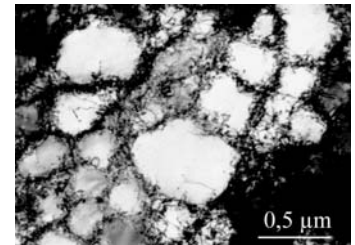
Below a critical dislocation density, the Helmholtz free energy of cell structure is higher than that of homogeneous distribution so that cell structure will not form at a low dislocation density case.

## Experimental microstructures

In the small strain regime the dislocations are distributed homogeneously. As deformation progresses, dislocation density is increased and cells are formed



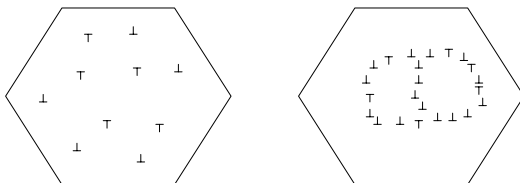
Low dislocation density  
Homogeneous distribution



High dislocation density  
Dislocation cell structure

## Statistical mechanics modelling

### 2 D single grain modelling



Low dislocation density  
Schematic homogeneous distribution

High dislocation density  
Schematic cell structure

Free energy of homogeneous distribution: 
$$\sum_N U_H - Tk \ln \frac{P!}{(P-N)!N!}$$

Free energy of cell structure: 
$$\sum_N U_C - Tk \ln 2^{N-1}$$

$U_H$ : elastic energy of one dislocation in homogeneous distribution

$N$ : Total number of dislocations

$T$ : Temperature  $k$ : Boltzmann constant

$P$ : Total positions for dislocations  $P=A/(4b)^2$

$A$ : Grain area  $b$ : Burgers vector

$U_C$ : elastic energy of one dislocation in cell structure

## Future work

- Predict cell size considering combined effects of strain, strain rate and temperature.
- Investigate the effect of grain morphology.
- Study the combined effects of alloying, grain size distributions, texture, temperature and rolling schemes.

References:

1. P. E. J. Rivera Díaz del Castillo and S. van der Zwaag, "A statistical mechanics theory of grain deformation and its prediction of dynamical recovery and recrystallization", *Materials Science Forum*, 467-470 (2004), 87-92.
2. P. E. J. Rivera Díaz del Castillo, M. Huang, S. van der Zwaag, Statistical mechanics prediction of solid-solid transformations induced by plastic deformation. Solid-Solid Phase Transformations in Inorganic Materials 2005 Conference. Phoenix, Arizona, USA, May 29-June 3, 2005.