Atomistic Simulation of Dislocations in Mg & Mg-alloys

Interaction between Yttrium clusters and dislocations

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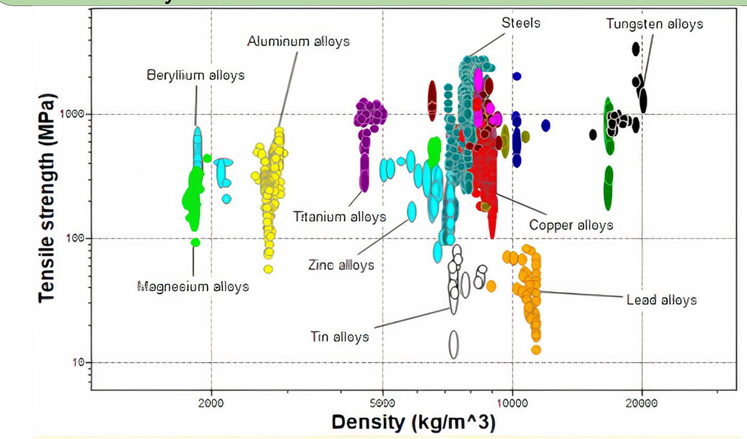
Motivation

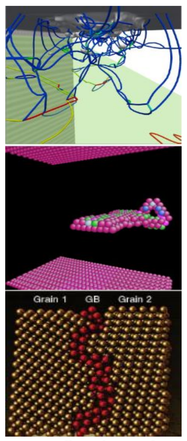
- Why Mg? - Lightweight, high strength
- Why Y? - Addition of Y lowers GSFE
- Why Clusters? - Possible new strengthening mechanism
- Issue with current Mg alloys? - low ductility, creep resistance, flammability etc.



Methods

Hybrid Molecular Dynamics/ Monte Carlo Simulation

Constant-Temperature MD



Simplified schematic of the molecular dynamics algorithm

Give atoms initial $\boldsymbol{r}^{(i=0)}$ and $\boldsymbol{v}^{(i=0)}$, set $\boldsymbol{a} = 0.0$, $t = 0.0$, $i = 0$, choose short Δt

Predictor stage: predict next atom positions:
Move atoms: $\boldsymbol{r}^p = \boldsymbol{r}^{(i)} + \boldsymbol{v}^{(i)}\,\Delta t + {}^1/_2\,\boldsymbol{a}\,\Delta\,t^2$ + more accurate terms
Update velocities: $\boldsymbol{v}^p = \boldsymbol{v}^{(i)} + \boldsymbol{a}\,\Delta t$ + more accurate terms

Get forces $\boldsymbol{F} = -\nabla\,V(\boldsymbol{r}^p)$ or $\boldsymbol{F} = \boldsymbol{F}(\,\Psi(\boldsymbol{r}^p)\,)$ and $\boldsymbol{a} = \boldsymbol{F}/m$

Corrector stage: adjust atom positions based on new $\boldsymbol{a}$:
Move atoms: $\boldsymbol{r}^{(i+1)} = \boldsymbol{r}^p$ + *some function of* $(\boldsymbol{a}, \Delta t)$
Update velocities: $\boldsymbol{v}^{(i+1)} = \boldsymbol{v}^p$ + *some function of* $(\boldsymbol{a}, \Delta t)$

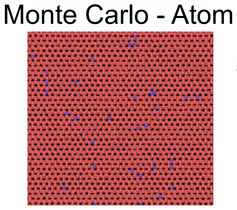
Apply boundary conditions, temperature and pressure control as needed

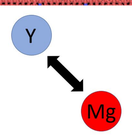
Calculate and output physical quantities of interest

Move time and iteration step forward: $t = t + \Delta t$, $i = i + 1$

Repeat as long as you need

Monte Carlo - Atom Swap (Metropolis method)





Algorithm 2 (Attempt to Displace a Particle)

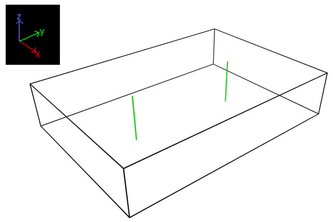
```
SUBROUTINE mcmove                    attempts to displace a particle

o=int(ranf()*npart)+1                select a particle at random
call ener(x(o),eno)                  energy old configuration
xn=x(o)+(ranf()-0.5)*delx            give particle random displacement
call ener(xn,enn)                    energy new configuration
if (ranf().lt.exp(-beta              acceptance rule (3.2.1)
+   *(enn-eno)) x(o)=xn              accepted: replace x(o) by xn
return
end
```

Workflow

General Goal	Example Specific Goal
Observe clusters in bulk Mg	Hybrid MC/MD simulation in Semi-Grand Canonical ensemble
Introduce dislocations	Consistent Stacking Fault width among MD/DFT/experiments
Integrate above two steps	Confirm solute-solute interaction between Mg and Y
Apply different external conditions (stress/temperature etc.)	Validation of σ - ε curve

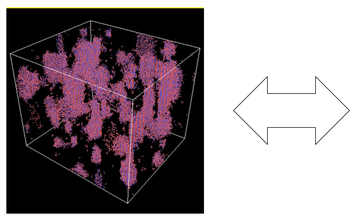
Simulation Setup

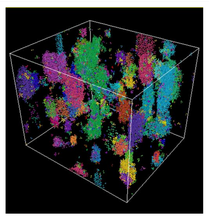


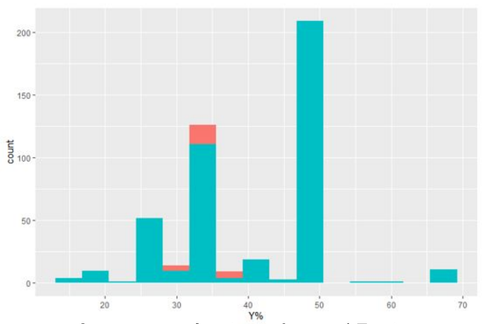
- 2 screw dislocations
- Dimension: 15.5 (x) * 22.1 (y) *4.7 (z) nm
- Distance between 2 dislocation lines: 11nm
- EAM potential
- Hybrid MC/MD (ratio of 1:50)
- 300K

Preliminary Results

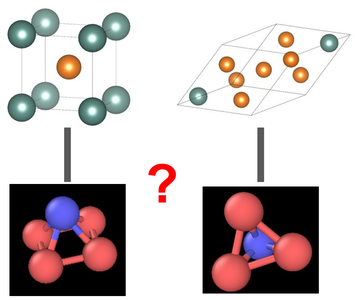
Red - Mg
Blue - Y



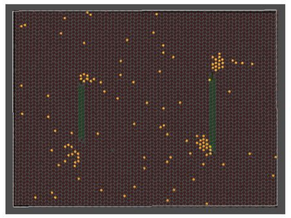


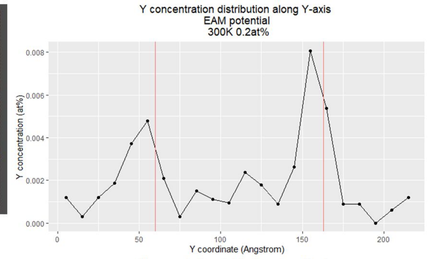


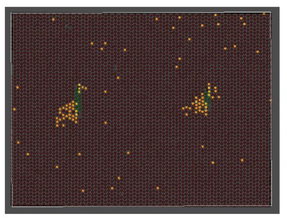
Average cluster size - 15 atoms
Large > 15 atoms
Small < 15 atoms

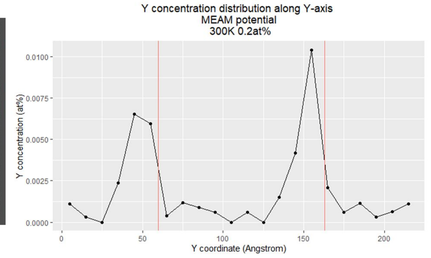


MgY Mg2Y









- Critical Y concentration (to form clusters):
  Bulk EAM: 0.3 at%
  Bulk MEAM: 0.2 at%
  Defect EAM: 0.1 at%
  Defect MEAM: 0.1 at%

Future Work

- Apply external conditions
- Look for solute segregation & interaction model

Long Term Goal

Further simulations with applied shear stress & different temperature

Purpose non-Rare Earth element as replacement for Yttrium

Design cheap & ductile Mg-alloy

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