Modeling of solidification in nano-scale

Molecular dynamics for alloying process

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Overview

Overview

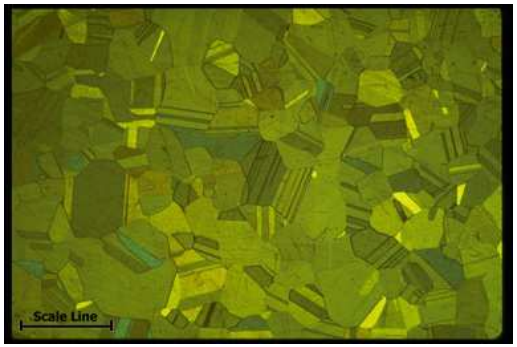
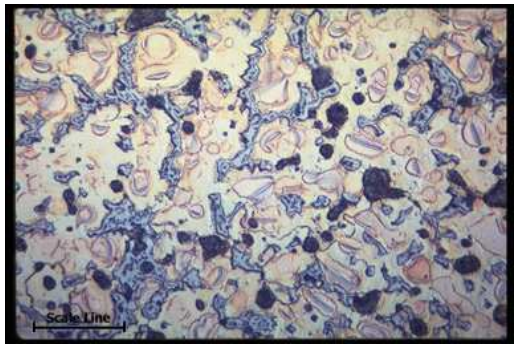
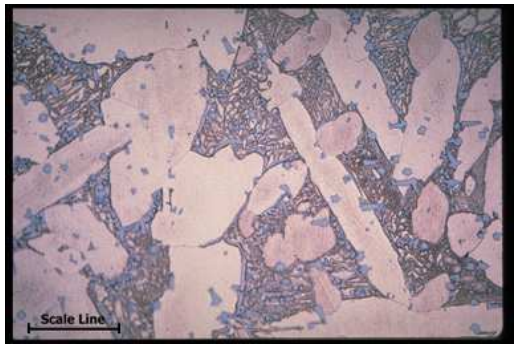
Structures in alloys

The various structures present in alloys are:

- the macro-structure ($\sim$10 μm) gives configuration of the constituents of alloys $\longrightarrow$ dendrite growth
- different crystal configuration for each constituents
- the temperature of solidification T_f – solidification can be quite complex (solidus-liquidus)

Alloy macro-structure

www.copper.org

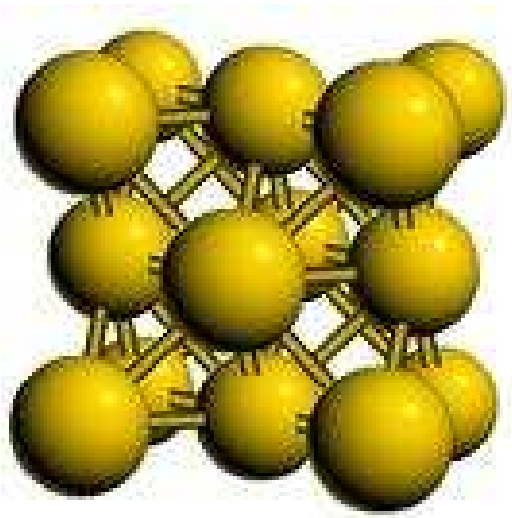
copper alloy	Cu 80%, Pb 8%, Sn 10%, Zn 0.5%, Ni 1%, S 0.5%	Cu 35.8%, Al 10.2%, Fe 4.0%
		
0.5 mm	25 μm	50 μm

Examples of alloy macro-structures

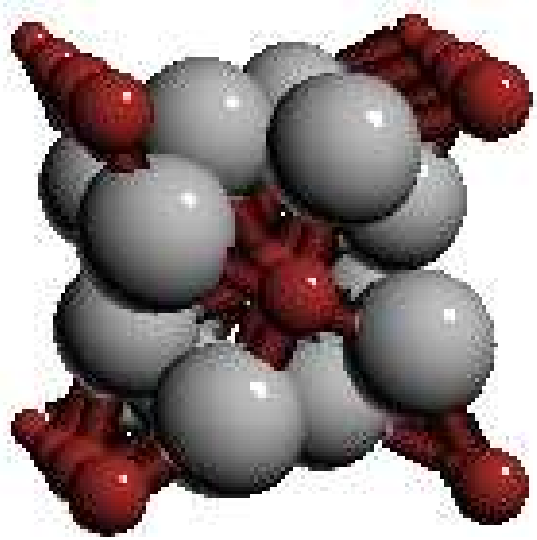
Crystal structure

cst-www.nrl.navy.mil/lattice

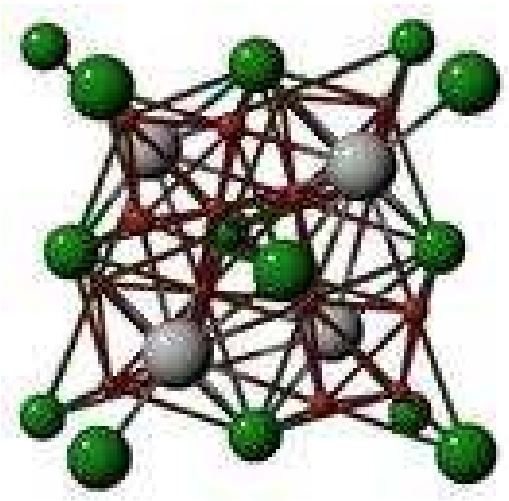
ccf crystal (Al)



Al_2Cu



$MgSnCu_4$



Examples of crystals

Examples of alloys

Most common alloys

- bronze (Cu + Sn)
- steel (Fe + C)
- aluminum alloys (Al + Cu, Si, Mg, Zn, Ti, B, Sb, Na, Sr, Fe)

Properties of alloy composition

The rate of the constituents and the conditions of solidification have an impact on:

- mechanical properties (elasticity, solidity)
- electrostatic/electric properties
- temperature of fusion
- resistance to corrosion
- behavior under manufacturing processes (cutting, molding)

Aluminum alloys

Pure aluminum:

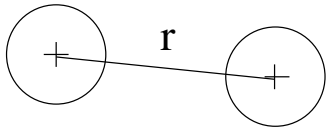
- it forms a cubic centered face crystal,
- it forms a thin impermeable layer at its surface.
- it is a ductile, light material

Possibilities of alloying aluminum are:

- + Mg $\rightarrow$ improves mechanical properties, most used alloying element for Al.
- + Cu $\rightarrow$ improves mechanical properties, repulsive to aquatic life.
- + Si $\rightarrow$ for complex molds
- + Sb or Na or Sr $\rightarrow$ used in Al-Si alloys, modifies the eutectic growth, not to be mixed!

Overview

Lennard-Jones potential



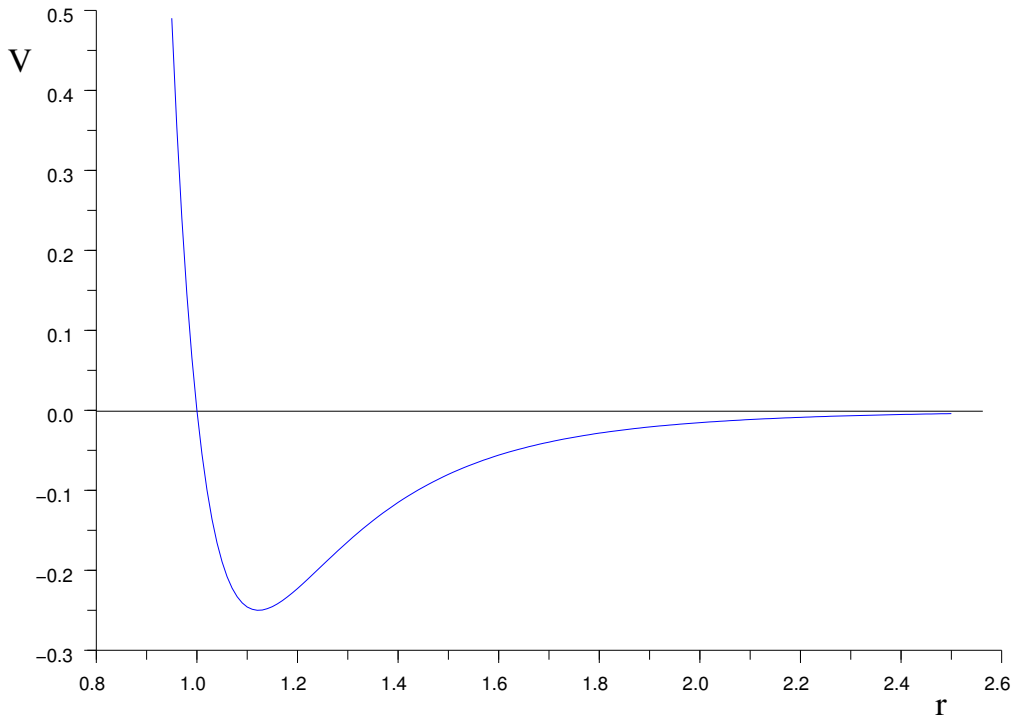
One-to-one interaction model with the potential:

$$V(r) = \varepsilon \left(\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right)$$

Two different potentials:

- a pair potential to account for the repulsion resulting from Pauli's exclusion principle,
- and the local electronic density accounting for cohesion.

Lennard-Jones potential



minimum at $r = \sigma_0 = 2^{1/6}\sigma$

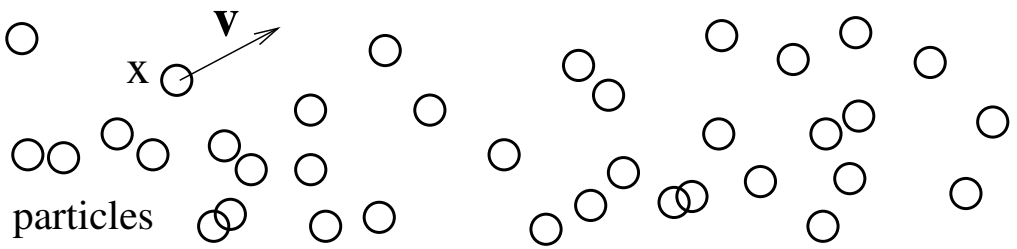
Lennard-Jones model properties

Lennard-Jones model:

- Interactions between spherical non polar particles,
- Very good model for noble gas,
- Good model for liquids,
- simple $\Longrightarrow$ fast and robust.

Overview

Atoms are modeled by interacting points.



Verlet algorithm:

$$\mathbf{x}(t+\delta t) = 2\mathbf{x}(t) - \mathbf{x}(t-\delta t) + \frac{\mathbf{f}(t)}{m}\delta t^2 + O(\delta t^4)$$

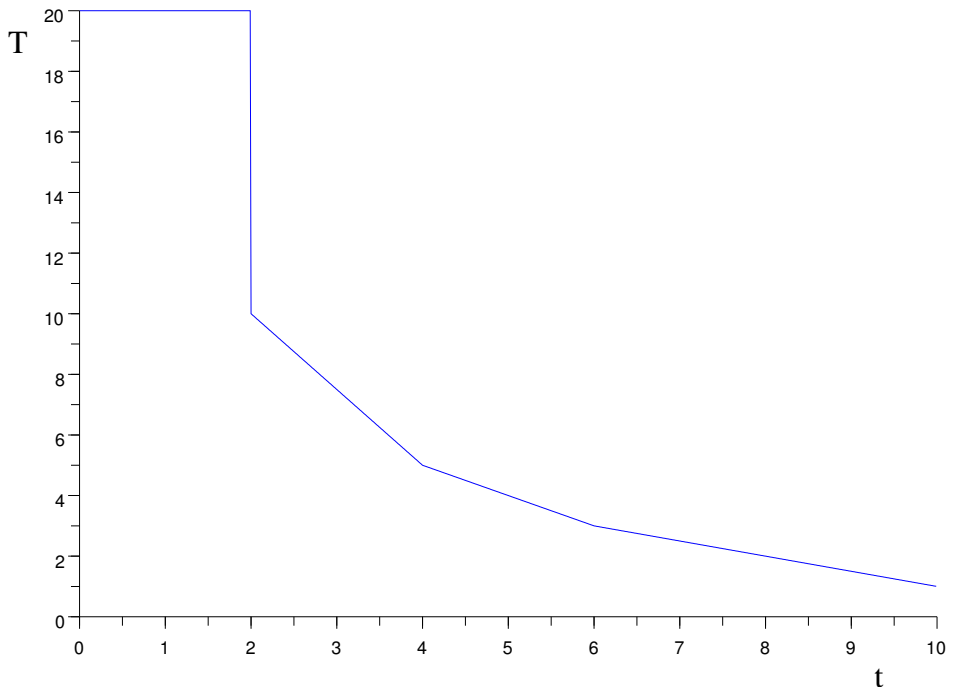
with $\mathbf{f} = -\nabla V$

http://lammps.sandia.gov

Overview

Crystallization box

In a periodic box, we fix the volume V, the density ρ, the rates of each kinds of atoms, and the evolution of the temperature.



We observe the crystallization process and the resulting structures of the alloys.

Crystallization box

Numerical experiment figures:

- 4 000 atoms,
- 200 000 time steps,
- $\sim$2 hours of computing.

Overview

Lennard-Jones parameters

- energy of the link ε,
- specific distance of interaction σ from:

$$V(r) = \varepsilon \left(\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right)$$

- mass m of the atom,
- density ρ of atoms in the box.

From ρ and σ we define the compactness $\kappa = \rho\sigma^3$.

Lennard-Jones parameter calibration

Then we obtain numerically:

- the mass per volume $M = \rho m$
- the temperature of fusion $T_f = \varepsilon f(\kappa)$
- the pressure $P = P(\kappa, \sigma, \varepsilon, m, T)$

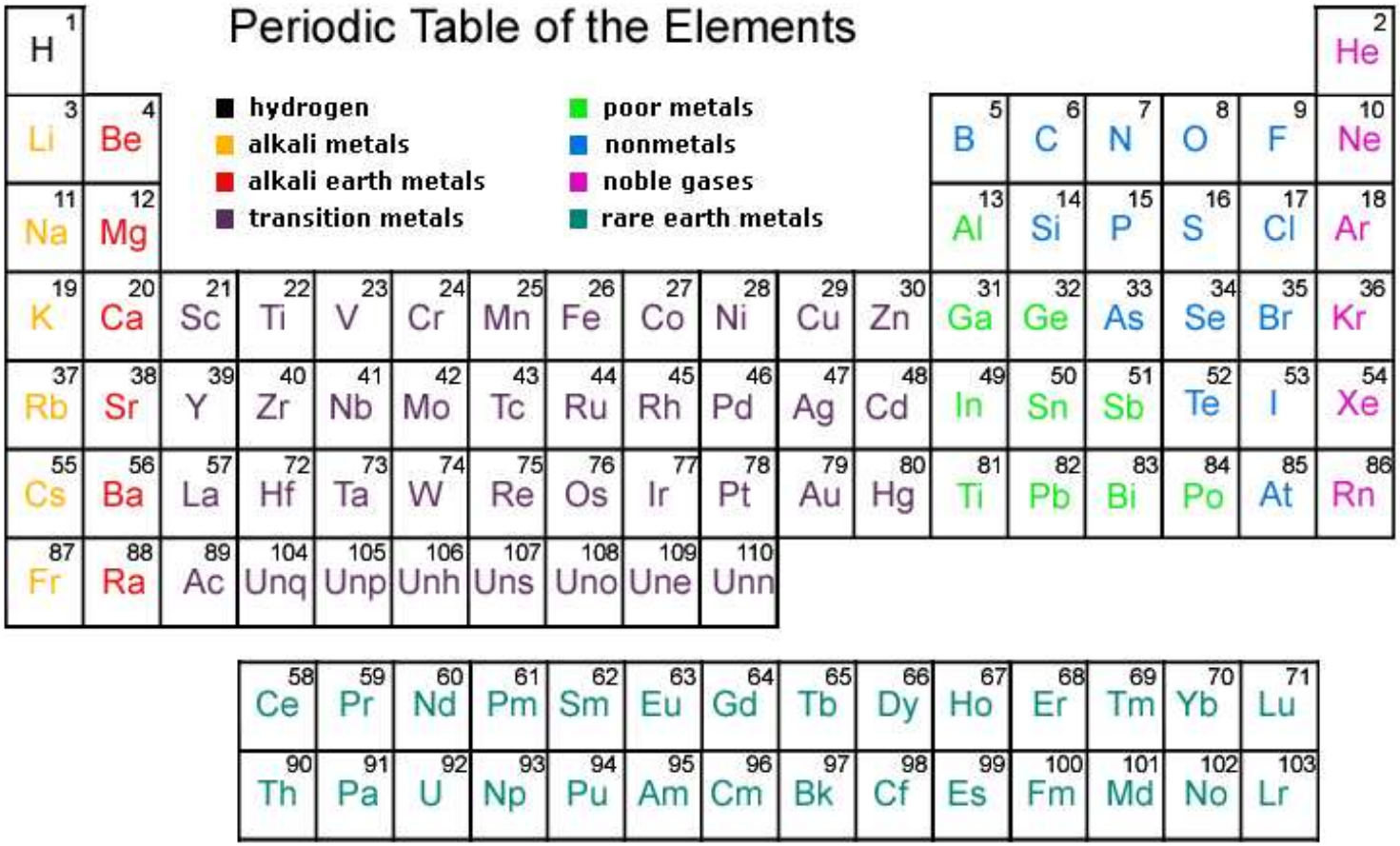
Overview

LJ approximation of Al, Cu, Sn and Mg

We simulate Al, Cu, Sn and Mg atoms which have the following properties:

	Al	Cu	Sn	Mg
m (g/mol)	27.0	63.6	118.7	24.3
M (kg/m^3)	2719	8978	7310	1738
T_f (K)	934	1358	505	923

Periodic table



LJ parameters for Al, Cu, Sn and Mg

	Al	Cu	Sn	Mg
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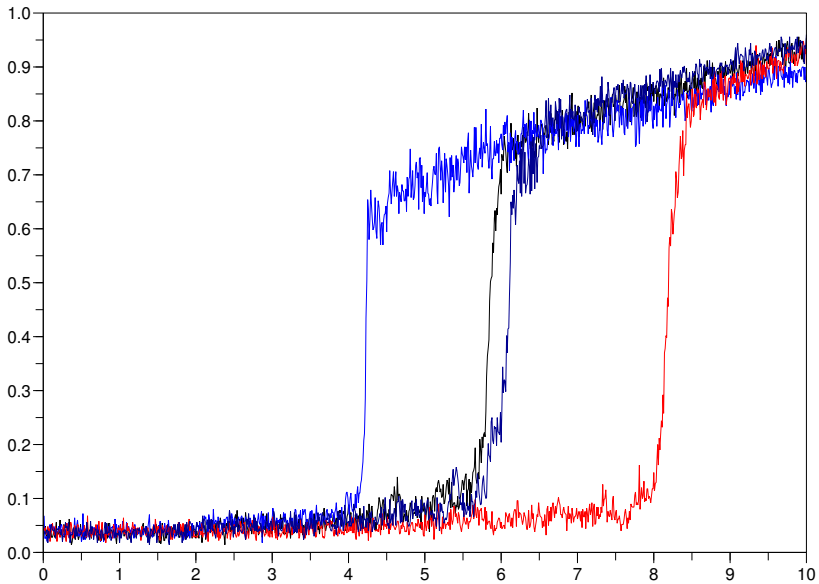
gives

	Al	Cu	Sn	Mg
ε	2.748	4.715	0.504	2.027
σ	1.1336	1.0023	1.4554	1.2977
ρ	0.7654	1.0726	0.46787	0.5435
κ	1.1150	1.0800	1.4424	1.1877

Solidification of pure Al, Cu, Sn and Mg

	Al	Cu	Sn	Mg
T_f (K)	934	1358	505	923



Rate of crystallization during time for Al (in black), Cu (in blue), Sn (in red) and Mg (in dark blue).

Overview

Crystal lattice

In a crystal, atoms are located at:

$$\mathbf{x}_\lambda = a\lambda_1\mathbf{e}_1 + a\lambda_2\mathbf{e}_2 + a\lambda_3\mathbf{e}_3 \qquad \text{with} \quad \lambda \in \mathbb{Z}^3$$

for some basis $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ of $\mathbb{R}^3$.

In cubic centered-face, each atoms A have 12 neighbors A_i, and the next closest atoms are at a distance of $\sqrt{2}a$ of A.

We take $\mathbf{e}_i = \vec{AA}_i$. We write all atoms B in a neighborhood $N(A)$ of A such that $d(A, B) \leq 3a$, in the $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ coordinates centered on A:

$$\vec{AB} = x_1(B)\vec{AA}_1 + x_2(B)\vec{AA}_2 + x_3(B)\vec{AA}_3$$

Crystal lattice

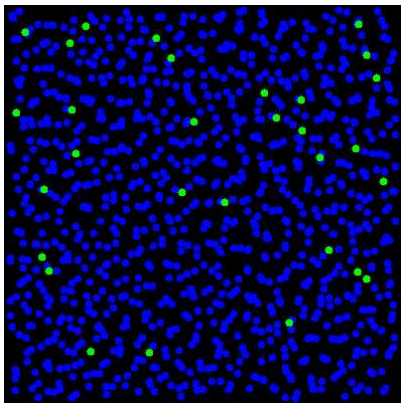
Then we compute the criterion μ:

$$\mu = \frac{1}{\#N(A)} \sum_{B \in N(A)} \frac{1}{3} \left(\cos(2\pi x_1(B)) + \cos(2\pi x_2(B)) + \cos(2\pi x_3(B)) \right)$$

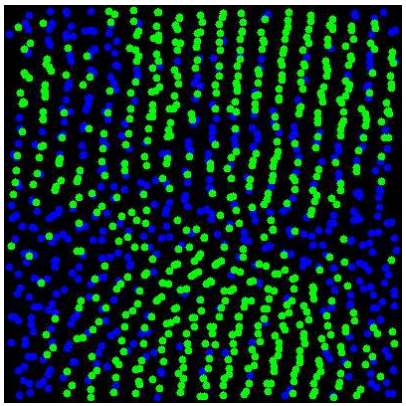
If $\mu \geq \mu_0$ (with $\mu_0 \approx 0.5$), A is considered as being inside a crystal structure.

Cu crystallization

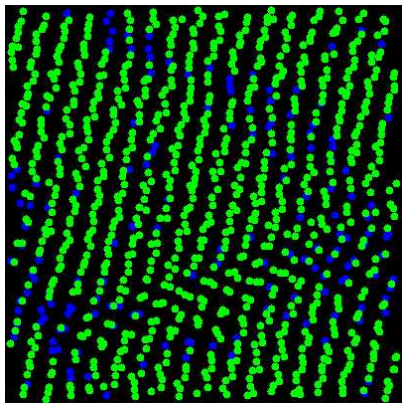
t = 0.3
T = 20



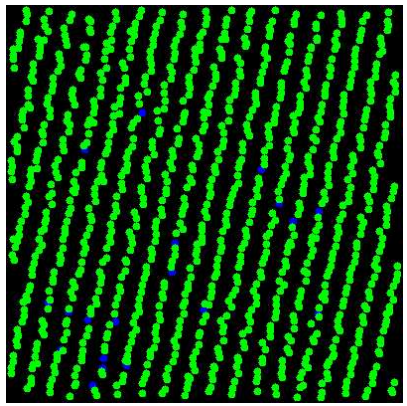
t = 4.7
T = 4.3



t = 5.4
T = 3.6



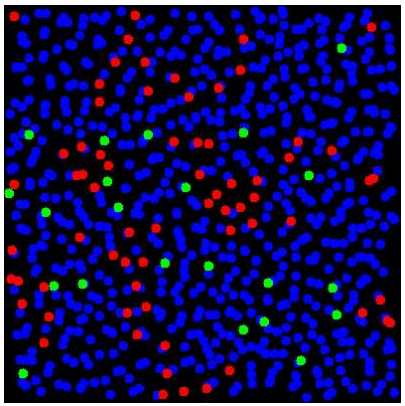
t = 6.3
T = 2.7



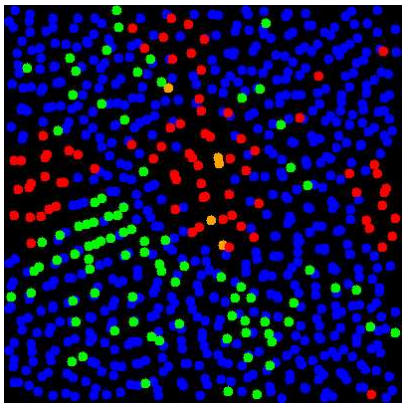
Solidification of LJ atoms with the Cu characteristics.
In blue: liquid atoms.
In green: ccf crystal atoms.

Cu-Sn crystallization

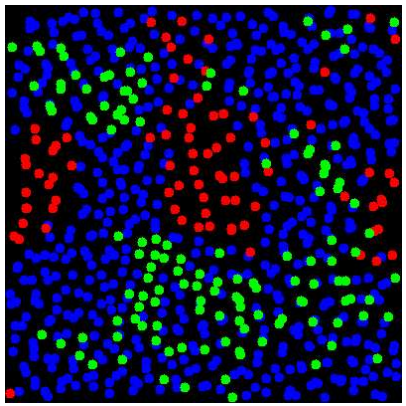
t = 1.5
T = 20



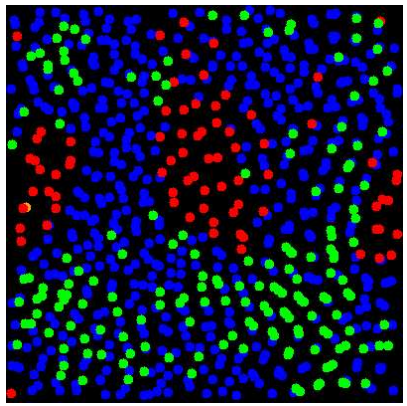
t = 5.2
T = 3.8



t = 6.2
T = 2.8

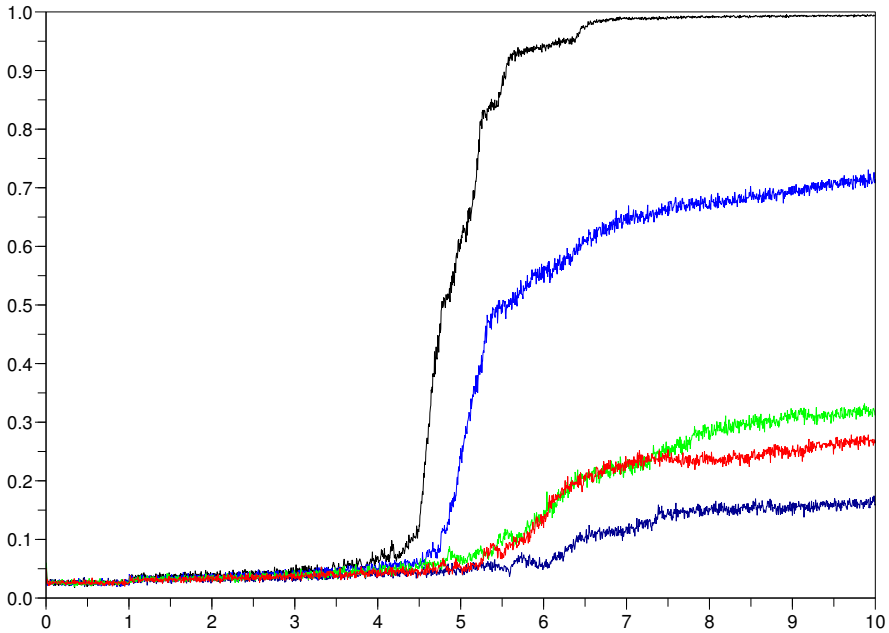


t = 9.9
T = 1.1



Solidification of LJ atoms with the Cu characteristics.
In blue: liquid Cu, in red: liquid Sn.
In green: ccf crystal Cu, in orange: ccf crystal Sn.

Comparison for various concentration in Cu-Sn alloys



Rate of ccf crystal locus for various concentrations in Sn:
$\rho_{\mathrm{Sn}} = 0,\ 0.05,\ 0.1,\ 0.15$ and 0.2

Overview

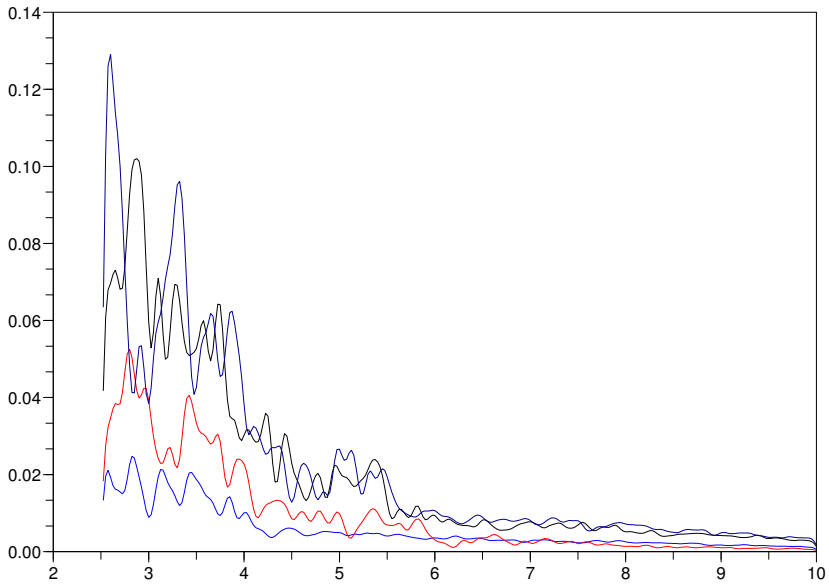
Green-Kubo diffusion

Green-Kubo formula:

$$D = \frac{1}{3} \int_0^\infty < \mathbf{v}(0) \cdot \mathbf{v}(t) > dt$$

where we noted $< y >$ the space average of y.

Diffusion for Al, Cu, Sn and Mg



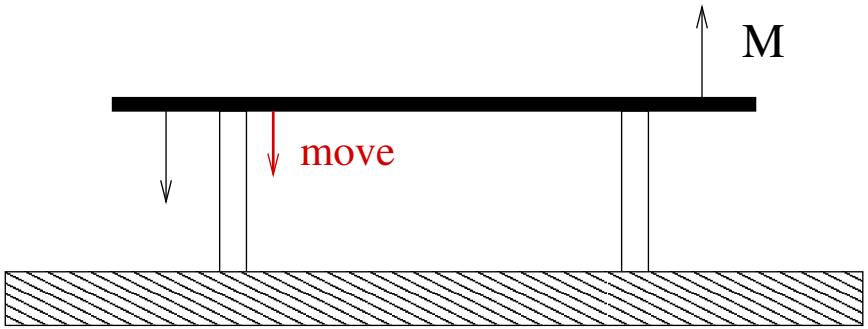
Noisy Green-Kubo diffusion computed for Al, Cu, Sn and Mg in the crystallization process.

Overview

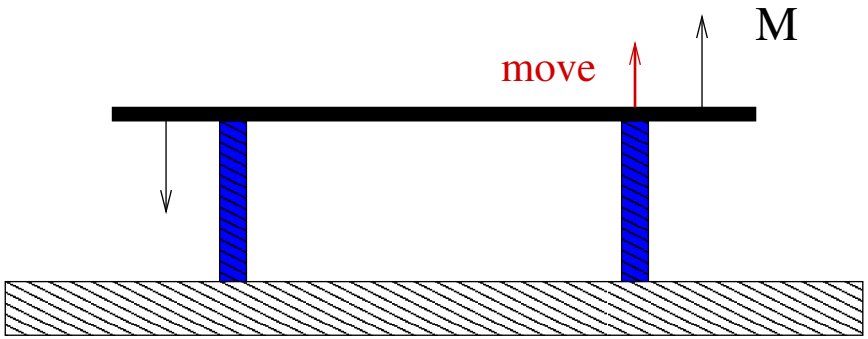
Mechanical properties of crystal

- big atoms (Sn) $\longrightarrow$ pressure force coherence
- small atoms (Cu) $\longrightarrow$ stirring force coherence

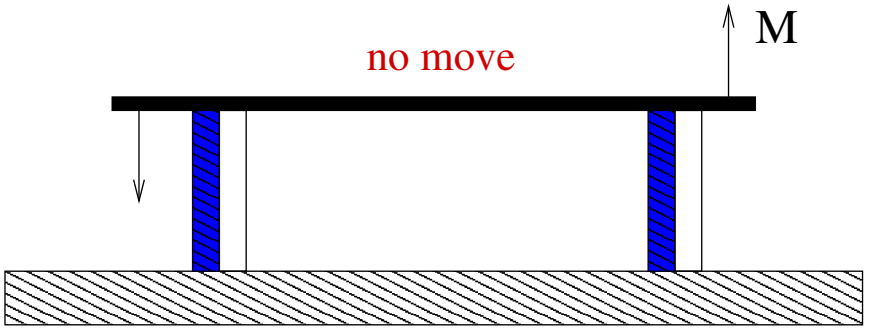
Alloying improvement



stirring resistant

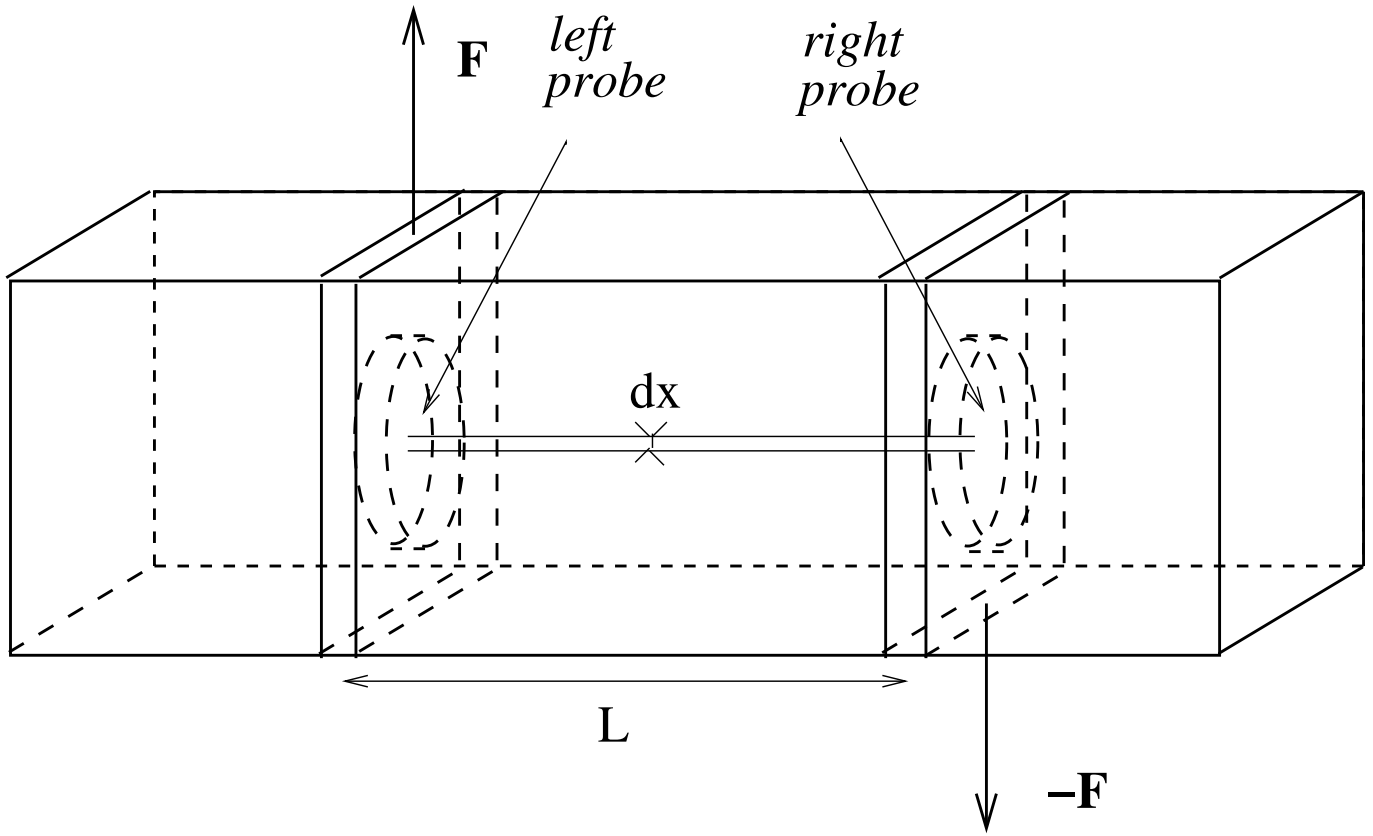


pressure resistant



resistant material

Experimental numerical test



periodic boundary conditions

Experimental numerical device to measure the deformation of a crystal under a shear stress force.

Elasticity

Stress $= F$

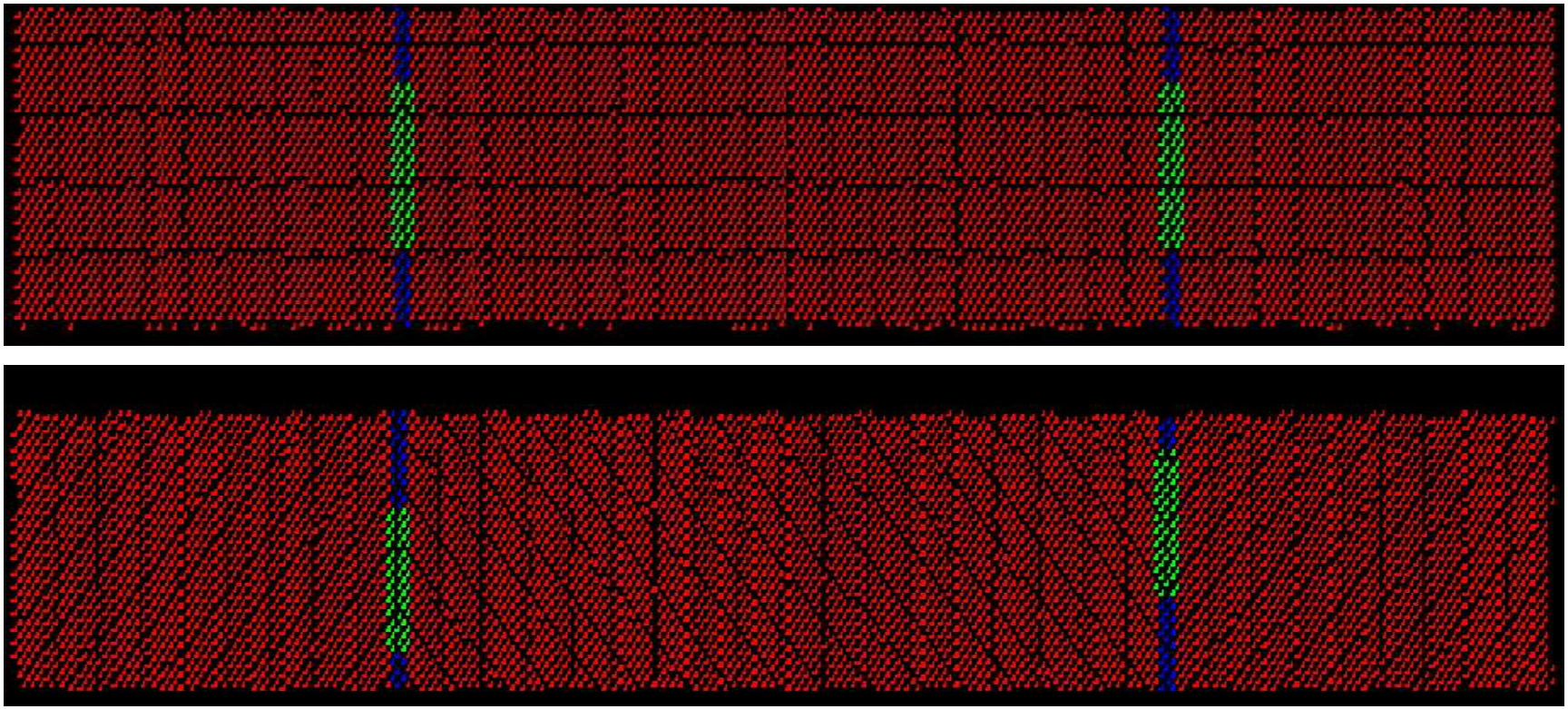
Strain $= \frac{dx}{L}$

Hence we obtain the following stress-strain relation:

$$\frac{dx}{L} = \alpha F$$

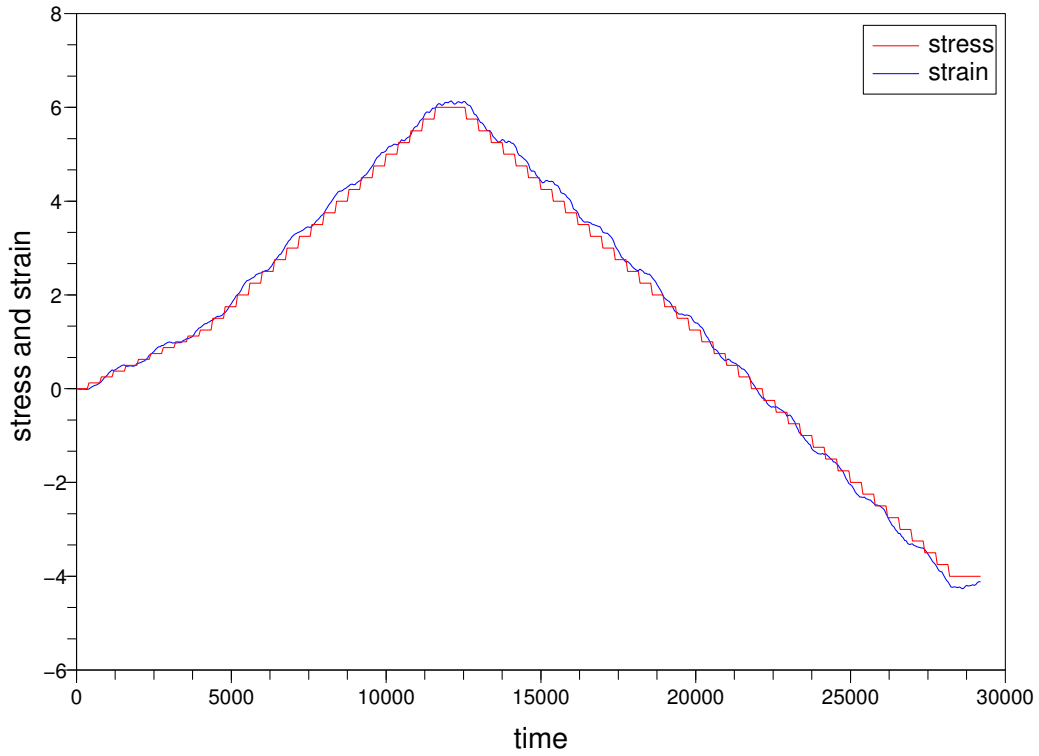
with α the elasticity constant of the material.

In practice



Location of the probes on the device (top). The material undergoes a shear stress (bottom).

Result for pure LJ crystal



Example of shear stress / strain deformation result for a crystal with Lennard-Jones potential model.

Conclusion

From solidification experiments we would like to:

- observe the segregation of atoms during the crystallization process,
- observe the variations on T_f depending on the concentration of alloying components,
- recreate the crystal structures of alloys,
- test for the mechanical properties.