# Simulation of the nucleation of the precipitate $Al_3Sc$ in an aluminum scandium alloy using Molecular Dynamics and kinetic Monte Carlo method

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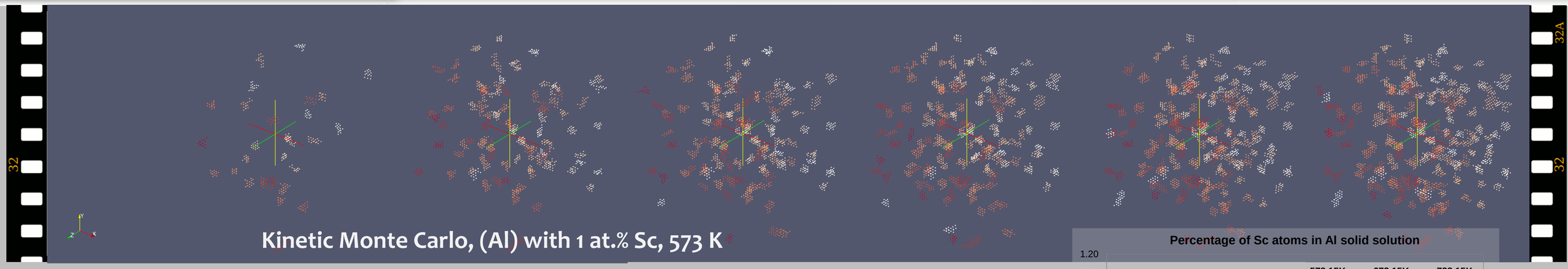
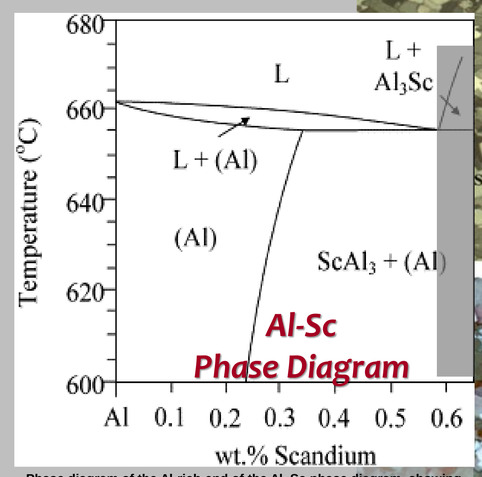
Functionalized Materials and Surfaces Performance



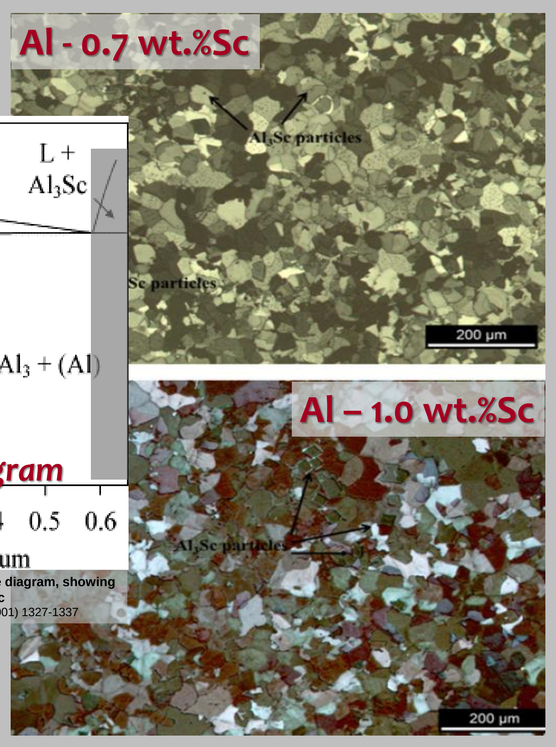

## Motivation

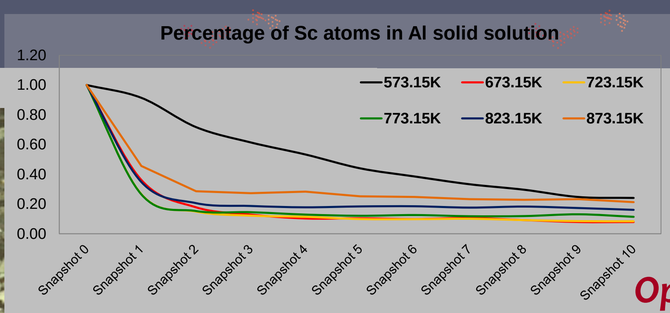
Low density, high strength to corrosion and specific strength to weight ratio are properties that made aluminum alloys excellent materials for transportation industry. A promising way to develop ultra-high strength aluminum alloys is achieved by the addition of metallic elements with low solubility in aluminum, promoting the $Al_3X$ (X = Sc) nanoparticles formation.
Moreover, Al alloys have applications in the aeronautic industry due to their enhanced mechanical properties if their specific strength to weight ratio is taken into account their specific strength to weight ratio. Our goal to study $Al_3Sc$ precipitates in Al alloys nucleation.

***Density Functional Theory (DFT), as implemented in VASP, and PHONON calculations were used to obtain several input parameters, like activation energies and attempt frequencies, to simulating $Al_3Sc$ nucleation using the kinetic Monte Carlo method. Quantum Molecular Dynamics was performed to characterize the diffusivity process.***
***The obtained results allow us to predict precipitates average size and radius over computational time, as well as the evaluation of the concentration of Sc in (Al) and precipitates density.***

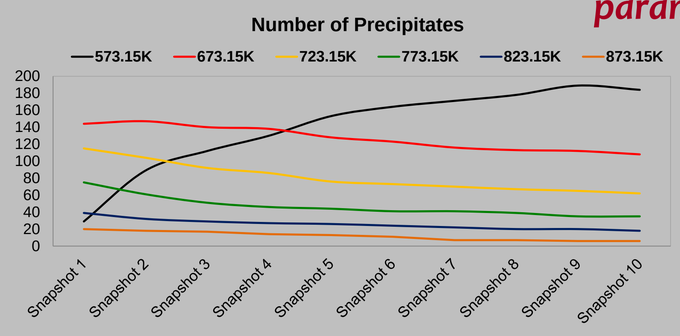


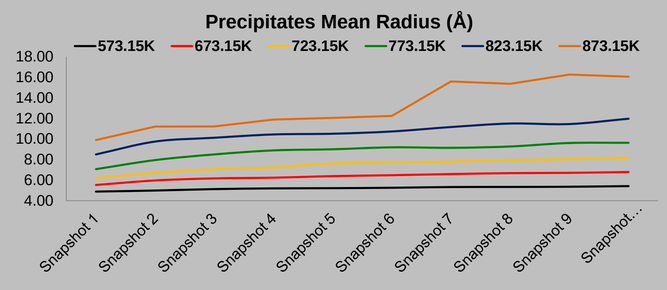

**Phase diagram of the Al-rich end of the Al–Sc phase diagram, showing a eutectic reaction at 0.55 wt. % Sc**
Hyde KB, Norman AF, Pragnell PB, Acta Mater 49 (2001) 1327-1337

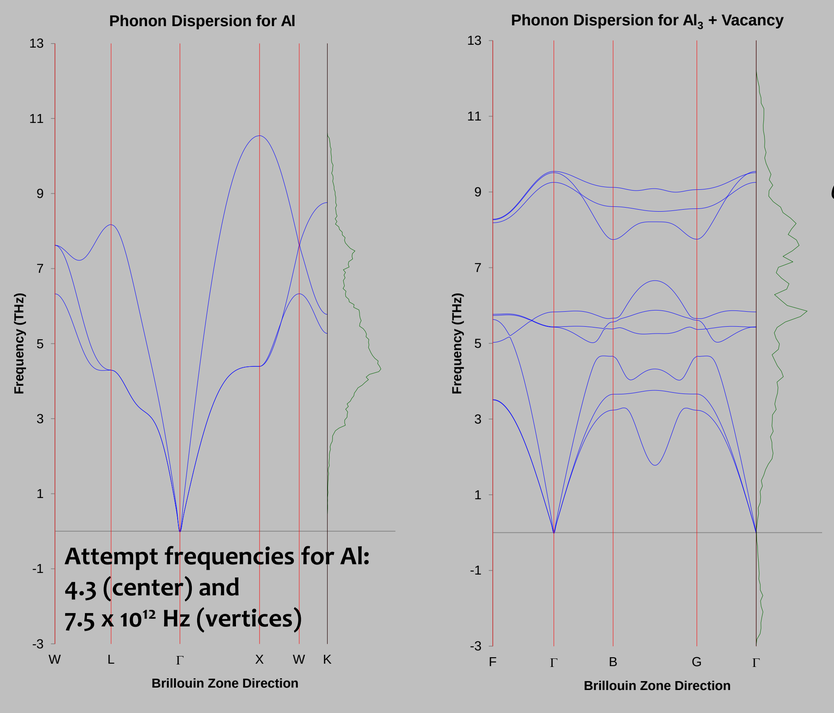



***Non Optimized parameters!***




**Attempt frequencies for Al:**
**4.3 (center) and**
**7.5 x $10^{12}$ Hz (vertices)**




## VASP – Mechanical Properties $Al_3Sc$

$$C_{ij} = \begin{vmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{vmatrix} = \begin{vmatrix} 164.46 & 34.35 & 34.35 & 0 & 0 & 0 \\ 34.35 & 164.46 & 34.35 & 0 & 0 & 0 \\ 34.35 & 34.35 & 164.46 & 0 & 0 & 0 \\ 0 & 0 & 0 & 52.95 & 0 & 0 \\ 0 & 0 & 0 & 0 & 52.95 & 0 \\ 0 & 0 & 0 & 0 & 0 & 52.95 \end{vmatrix} \text{ [Gpa]}$$

**Symbolic elastic constant matrix for a cubic system**

**VASP simulation of the elastic constants**

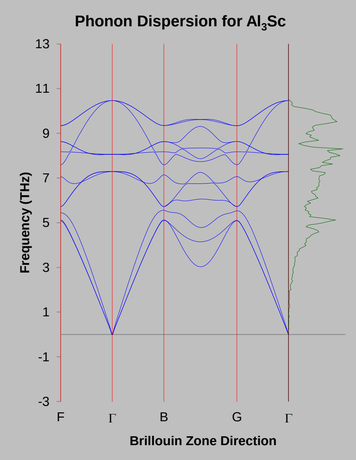
| Modulus | Voigt | Reuss | Hill |
|---|---|---|---|
| Bulk [Gpa] | 77.73 | 77.73 | 77.73 |
| Shear [Gpa] | 57.79 | 57.21 | 57.50 |
| Young´s [Gpa] | 138.95 | 137.82 | 138.38 |
| Longitudinal [Gpa] | | | 154.40 |

| Modulus | Al [1] | Al3Sc [2] | Al3Sc [3] |
|---|---|---|---|
| Bulk [Gpa] | 76.5 | 99 | 91.5 |
| Shear [Gpa] | 26.1 | 68 | 68.4 |
| Young´s [Gpa] | 70.3 | 166 | 164.2 |

[1]Meyers MA, Chawla KK, Mechanical of Materials, Prentice-Hall, Upper Saddle River, NJ (1999) 92
[2] George EP, Horton JA, Porter WD, Schneibel JH, J Mater Res 5 (1990) 1639
[3] Hyland Jr RW, Stiffler RC, Scripta Metall 25 (1991) 473

**MC inputs:**
Attemp frequencies √
Activation Energies
Pair effective energies

**Attempt frequency for Sc in Al3Sc:**
**5.5 x $10^{12}$ Hz**




## Conclusions

**We have calculated mechanical properties of Al3Sc, which are in good agreement with the experimental data from the literature.**

**We have calculated Phonon dispersion and density of states to obtain the attempt frequencies for Al and Sc.**

**We have performed MD in order to obtain diffusivity parameters for Al and Sc in an Al matrix.**

**We have made kinetic Monte Carlo simulations with non-optimized input parameters for method testing purposes.**

Ab Initio molecular dynamics (MD) simulations, under Born-Oppenheimer approximation were performed at elevated temperature (1800 K) to speed up diffusion and shorten the simulation time scale. The time step chosen was 2 fs.

With this data we will be able to calculate Al, Sc and Va diffusion coefficients. The diffusion coefficients will be calculated from the averaged mean square displacement of the atoms over time.
These values will be compared with the kinetic Monte Carlo output.

***Acknowledgements***

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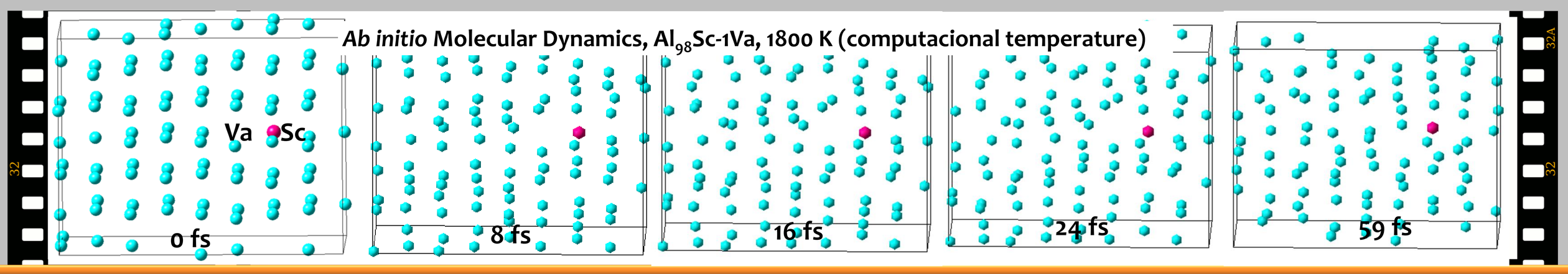
FCT, Portugal, for the financial support through project PTDC/CTM/68160/2006; PTDC/CTM/099461/2008 and SFRH/BD/87641/2012

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