Development of a specific N-body interatomic potential for modelling complex intermetallics with Molecular Dynamics

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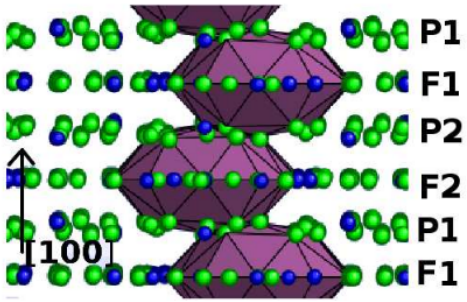
Content

- Introduction
- Principle - object of study
- Pure metals - algorithm reafinement
- Binary alloy AlCo
- Intermetallic complex $Al_{13}Co_4$
- Conclusion
- References

Introduction

Context

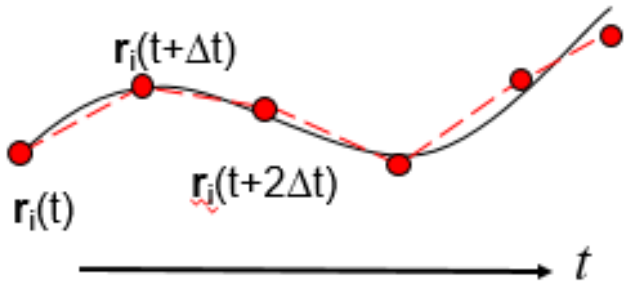
- Molecular deposit (fullerene) on metallic surface
- Quasi-crystal and approximant
- Large system $\rightarrow$ numerical computation
- Stability study by molecular dynamics $\rightarrow$ need interatomic potential



Introduction

Simulation of the structure by Molecular Dynamics

- Numerical integration of the equation of movement.
- Requires the analytic expression of interaction potential which gives us the expression of the forces
- $F_i = \frac{d \sum_i E_{ij}}{dr_i}$



- Will give us the dynamic evolution of our system

Principle - object of study

Second Moment Approximation - potential

- "SMA comes from Tight Binding theory"
- $U_i(r) = \sum_j A e^{-p(\frac{rij}{r_0}-1)} - \sum_j \sqrt{\xi^2 e^{-2q(\frac{r_{ij}}{r_0}-1)}}$
- 4 adjustable parameters A,p,q,ξ

Principle - object of study

Least square fitting

- Starting from data and equation supposed describing these data with free parameters
- $LS = \sum_i (U_i(r)_{exp} - U_i(r)_{calc})^2$
- Minimize LS by moving the free parameters

Principle - object of study

Intermetallic complex $Al_{13}Co_4$

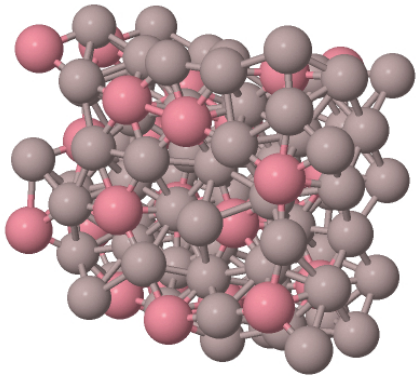


Figure: $Al_{13}Co_4$ structure

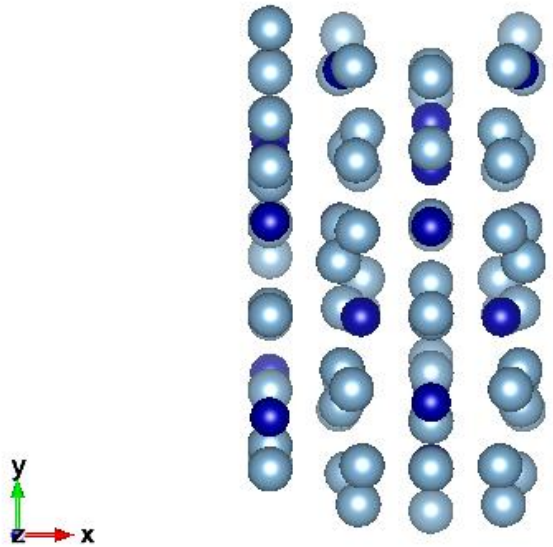


Figure: Profile view of $Al_{13}Co_4$ structure

- Alternating planes (Flat and Puckled) in the $Al_{13}Co_4$ structure
- 102 atomes in a (bx = 8.1 $\AA$, by = 12.3 $\AA$, bz = 14.4 $\AA$)

Pure Metals - algorithm reafinement

Fitting equation

- $U(x) = A.(12.e^{-p.(\frac{x}{r_0}-1)} + 6.e^{-p.(\frac{x.\sqrt{(2)}}{r_0}-1)})$
  $-\xi.\sqrt{12.e^{-2.q.(\frac{x}{r_0}-1)} + 6.e^{-2.q.(\frac{x.\sqrt{(2)}}{r_0}-1)}}$
- Al and Co are fcc structures
- r_0 first neighbor distance
- 6 first neighbors and 12 second neighbors

Pure Metals - algorithm reafinement

Choice for A,p,q,ξ parameters

- Find by hand the best interval in which the LS is minimize but also where compressibility data are recovered
- $A(p,q) = q.\frac{(12+6.\sqrt{2}.Q2).E_{coh}}{p.(12+6.\sqrt{2}.P2).(12+6.Q2)-q.(12+6.\sqrt{2}.Q2).(12+6.P2))}$
- $\xi(p,q) = p.\frac{(12+6.\sqrt{2}.P2).\sqrt{12+6.Q2}.E_{coh}}{p.(12+6.\sqrt{2}.P2).(12+6.Q2)-q.(12+6.\sqrt{2}.Q2).(12+6.P2))}$
- Numerical loop over p,q in the previous chosen interval.

Pure Metals - algorithm reafinement

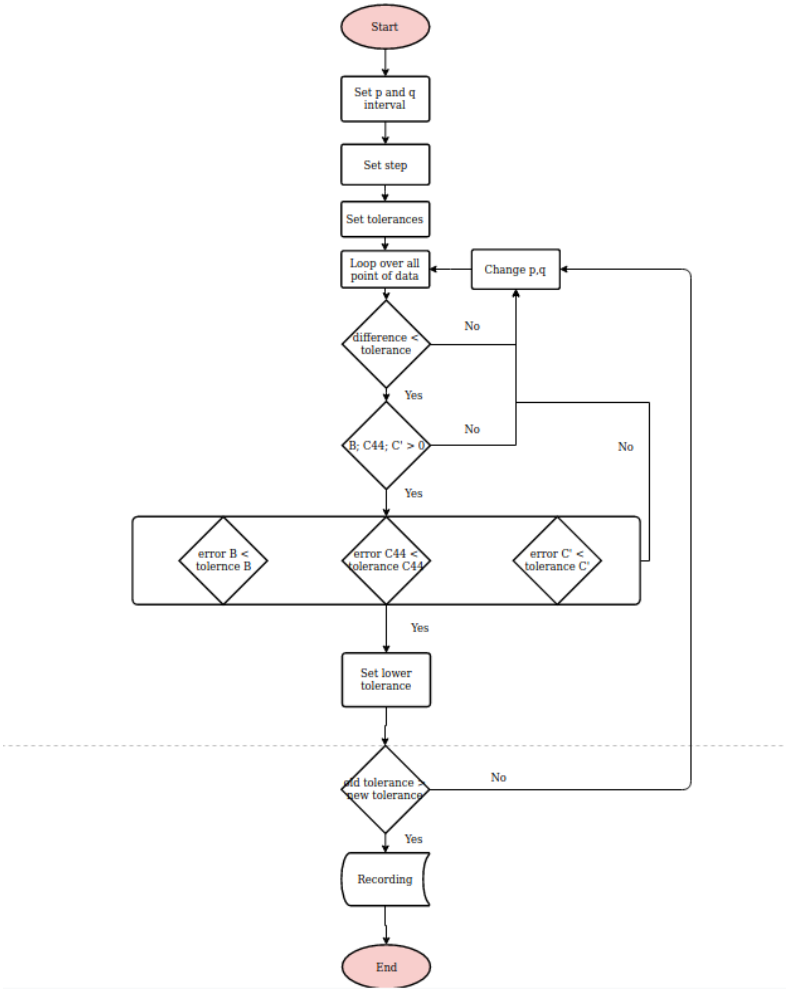
"Experimental" data

- Use of reference ab initio (DFT) curves for the total energy of bulk Al and Co
- Compressibility data like bulkmodulus B, shear modulus C44 and C'

Component	B (*Mbar*)	C44 (*Mbar*)	C' (*Mbar*)	E_{coh}(eV)	R_0(Å)
Al	0.77	0.33	0.26	3.49	2.85
Co	2.2	2.06	1.11	4.96	2.45

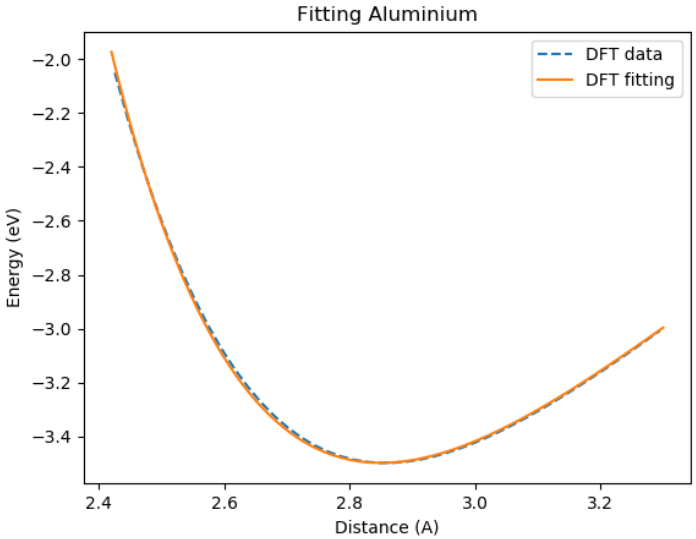
Pur Metals - algorithm reafinement

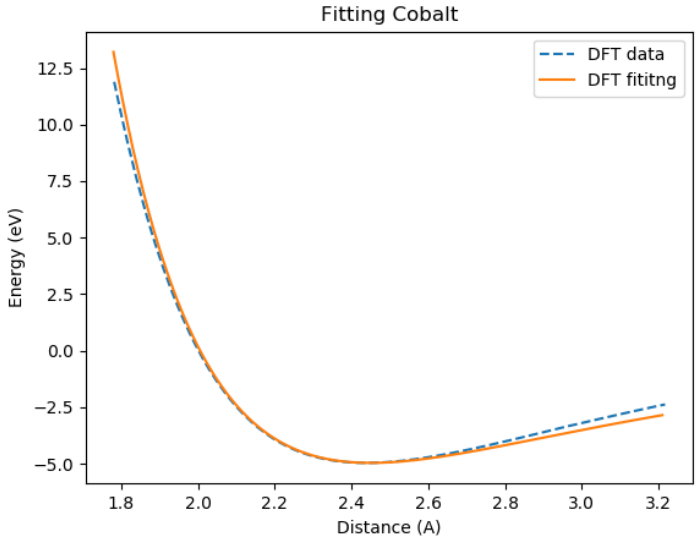
Algorigram



Pure Metals - algorithm reafinement

Results and comments





Component	B (*Mbar*)	C44 (*Mbar*)	C'(*Mbar*)
Al	0.77	0.45	0.13
Co	2.29	1.11	0.35

Component	A(eV)	p	q	ξ (eV)	LS
Al	0.85	9.41	2.08	1.25	0.0038
Co	0.17	9.55	2.74	1.97	2.62

Binary alloy

L_{10} structure

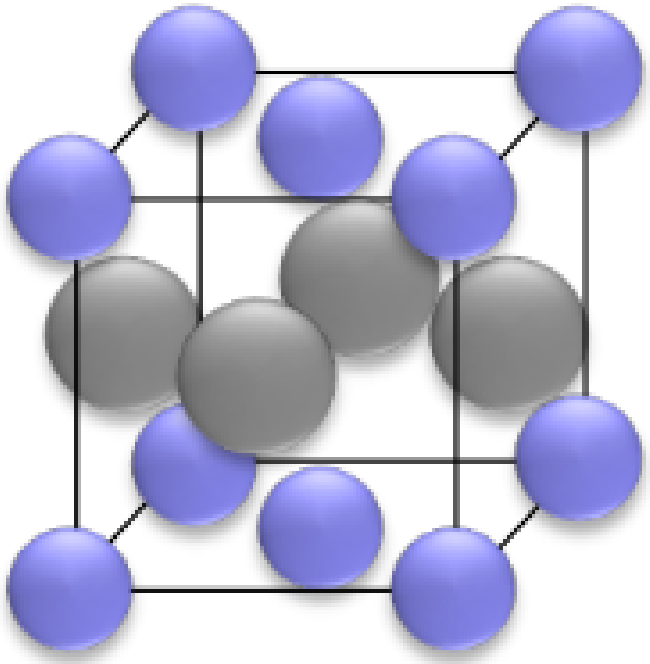


Figure: L_{10}

- Fcc based structure with different atom on central plane
- 50 % Al / 50% Co

Binary alloy

B_2 structure

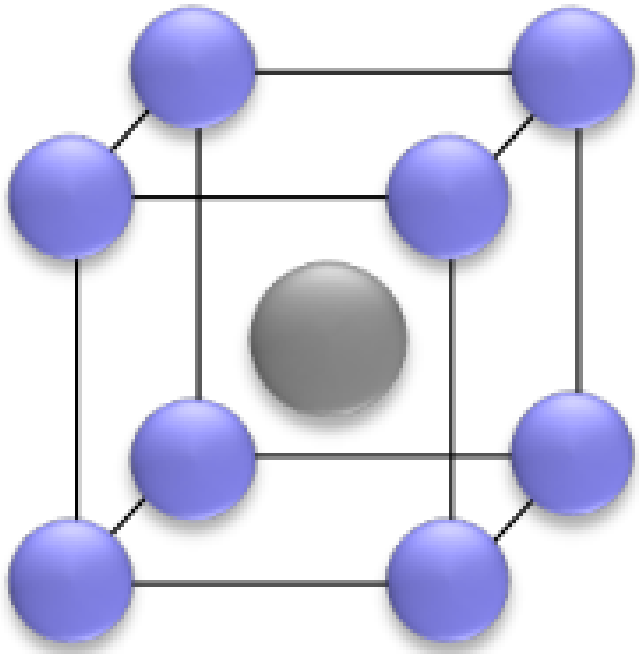
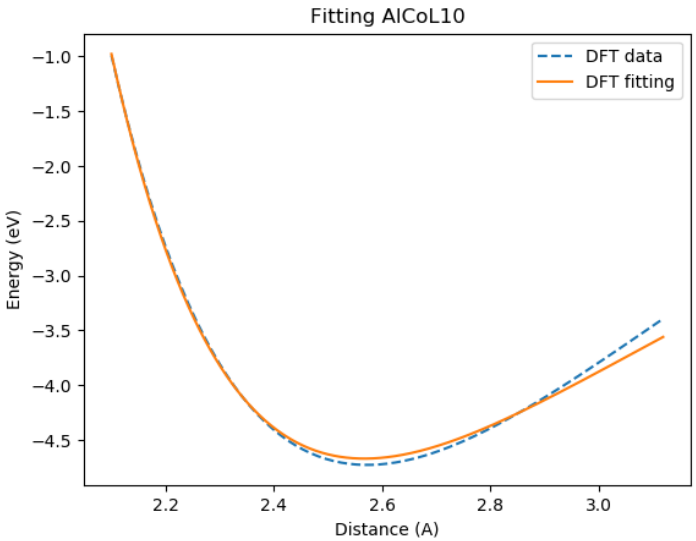


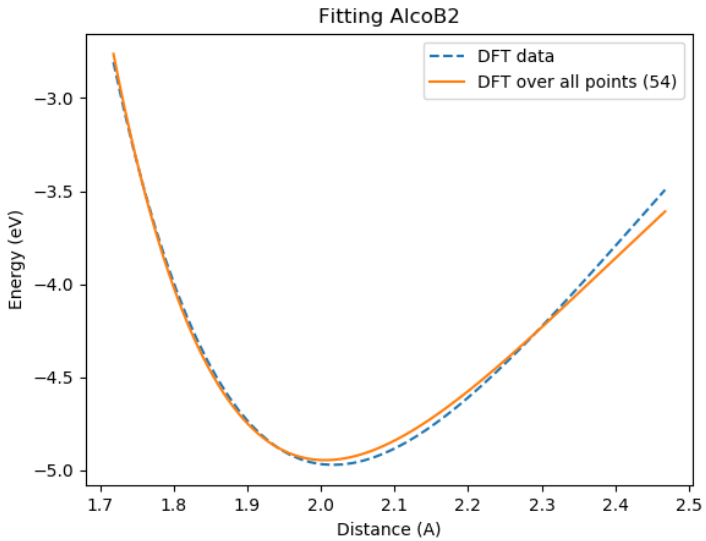
Figure: B2

- cc based structure with different atom on the center
- 50 % Al / 50% Co

Binary alloy

Results and comments





Parameters	A	p	q	ξ	LS
L10	0.095	9.48	2.41025	2.883	0.498594
B2	0.2001	9.48	2.41025	2.247	0.902769

Intermetallic complex $Al_{13}Co_4$

Stability control by Molecular Dynamics

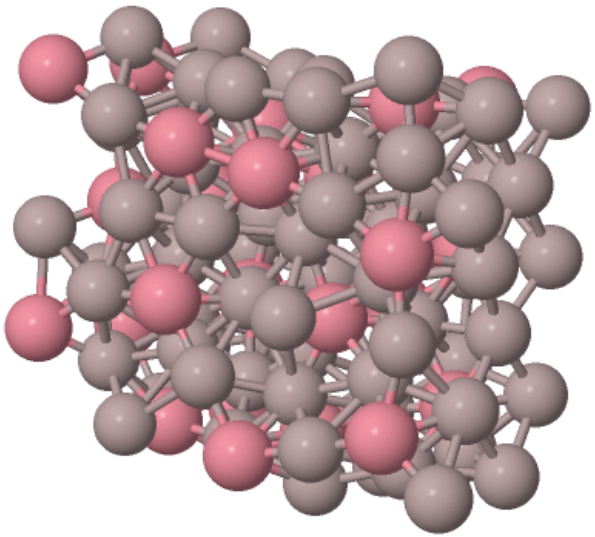


Figure: DFT

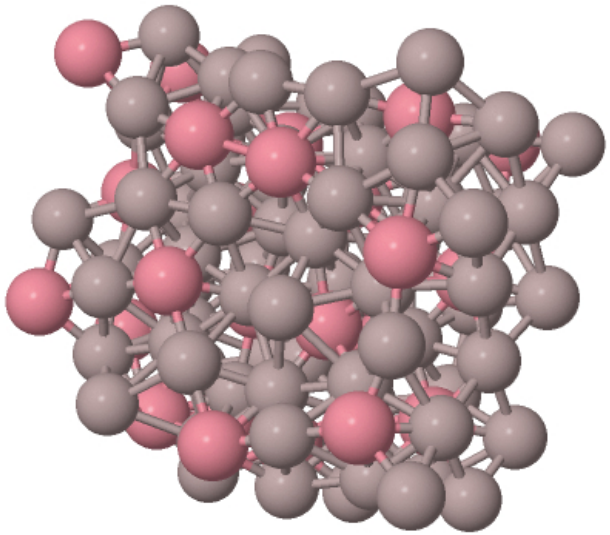
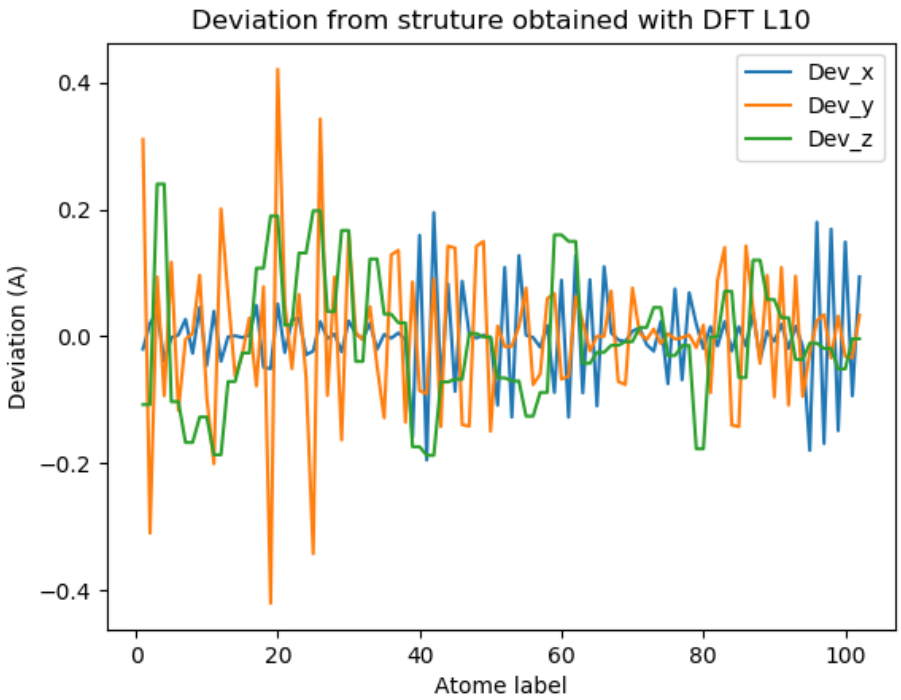


Figure: Molecular Dynamics

Intermetallic complex $Al_{13}Co_4$

Stability control by Molecular Dynamics



- Fluctuation $\rightarrow$ motion
- Reasonable $dev_{max} = \pm 0.4$

Conclusion

- Small deviation $\rightarrow$ stable structure
- Good reproducing of DFT energy curve
- Questionable reproducing of elastic constant

- $\rightarrow$ Seem available for deposit study of molecule on $Al_{13}Co_4$

Reference

- DFT curves and elastic constants, E.Gaudry from University of Lorraine
- Theorical aspects, "Étude par simulation numérique d'agrégats libres mono- et bi-métalliques" ,PhD thesis from M.C. Mottet, 1997, Univeristy of Aix-Marseille II
- DFT explanation, "Influence de la liaison chimique sur la structure des surfaces d'alliages métalliques complexes", PhD thesis from M. Meier, 2015, University of Lorraine
- $Al_{13}Co_4$ structure, PHYSICAL REVIEW B94, 165406 (2016)
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- Surface of a quasicrystalline approximant: Al 13 Co 4 (100) by É. Gaudry, C. Chatelier, D. Kandaskalov, L. Serkovic