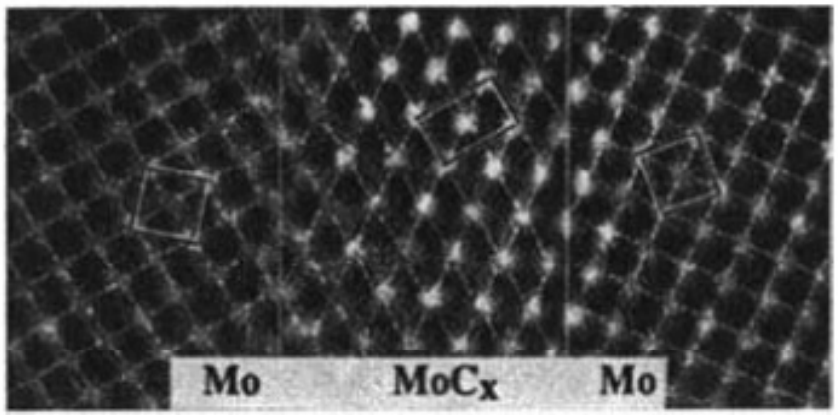
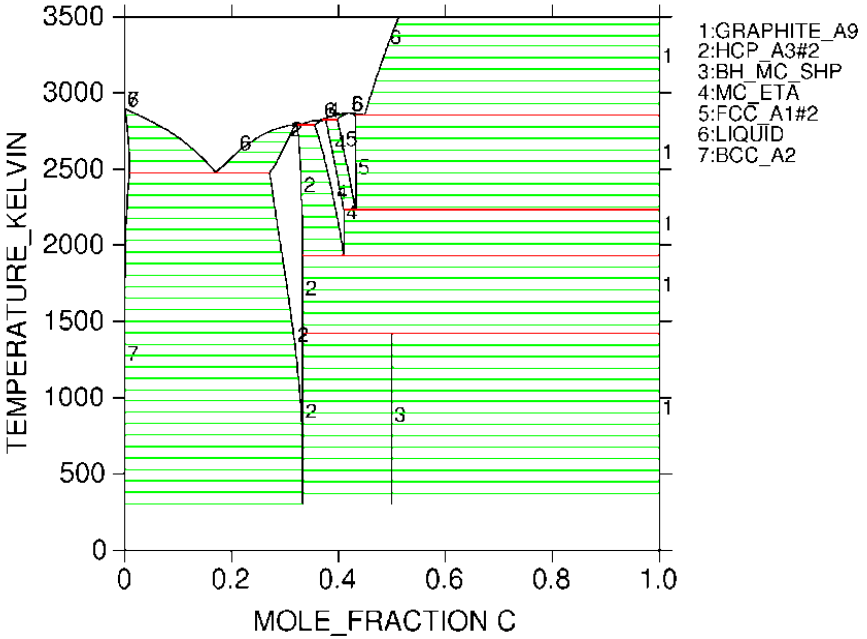




Absence of MoC_x phase in phase diagram. Why?

J.M. Penisson et.al
1996

Kramsach, 26.01.2012

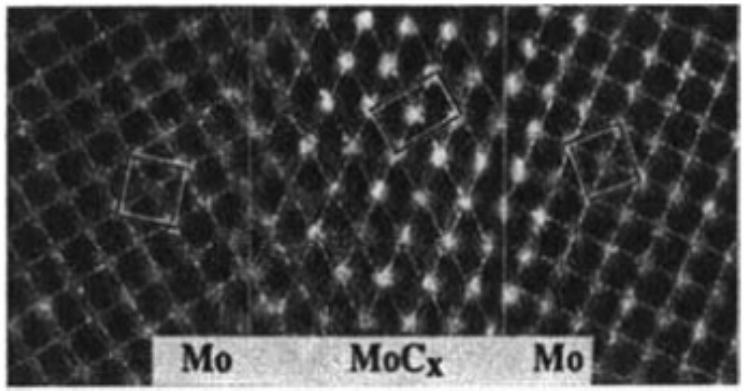
The role of coherency strain on the structural stability of a metastable precipitate in Mo-C binary system

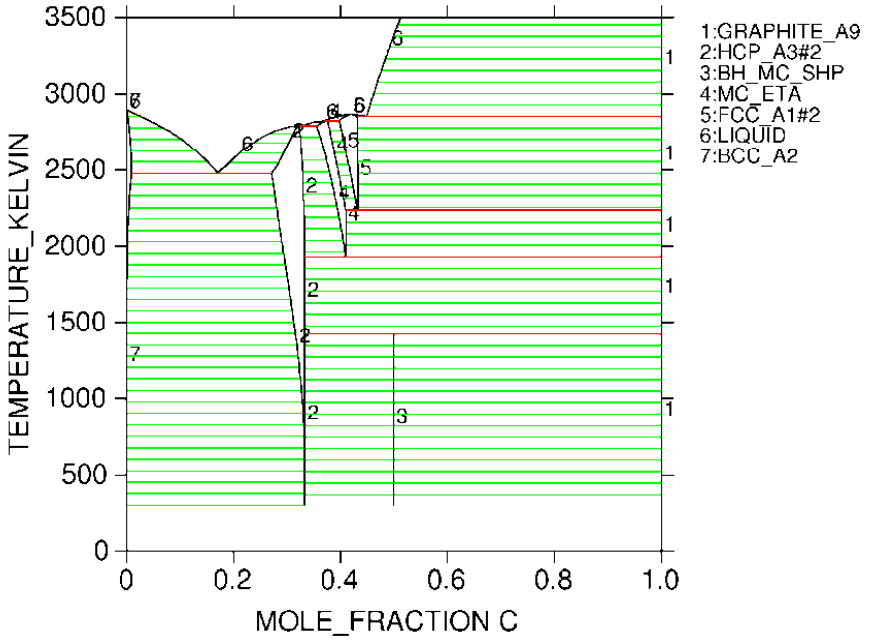
S.Sampath, R.Janisch, S.G.Fries, A.Hartmaier

Interdisciplinary Centre for Advanced Materials Simulation (ICAMS)
Ruhr-University Bochum, Germany

International Max Planck Research School for Surface and Interface Engineering in Advanced Materials (IMPRS SurMat)

Motivation





How it could be stabilized?

J.M. Penisson et.al
1996

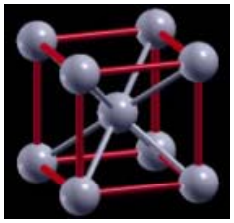
Structure of the talk

- Introduction
- Bulk study and their results
- Interface study and their results
- Summary

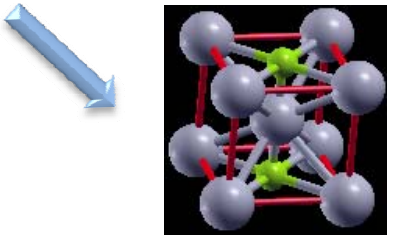
Technical details

- DFT calculations are being carried out using VASP code
- GGA for exchange-correlation effects
- UltraSoft pseudopotential for the core-valence interaction
- Electron wave function - Plane wave basis set – Cut-off energy
- K-point mesh – Monkhorst Pack type
- CALPHAD method by engaging Thermocalc software

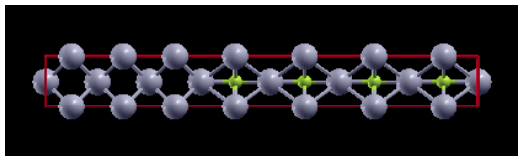
Introduction



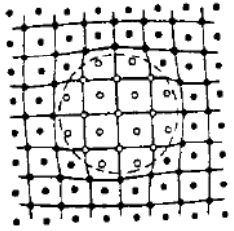
(Original matrix)



(Variation of lattice parameters)



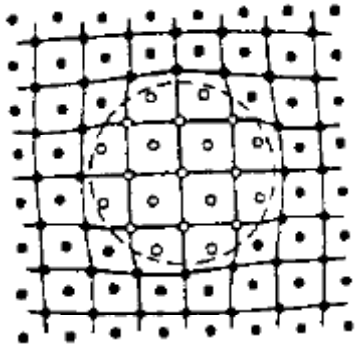
(Coherency strain)

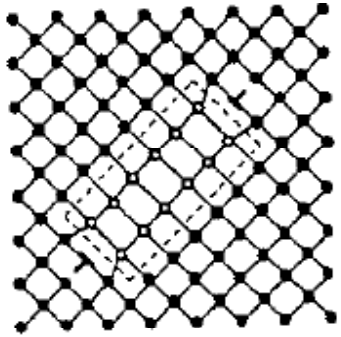


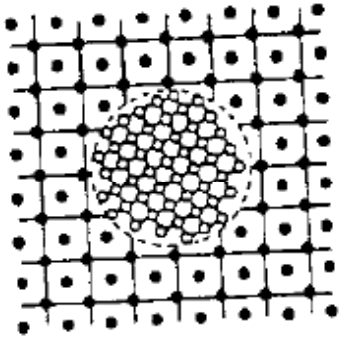
(Coherency of precipitate)

Interface energy?

Bulk study and their results







$$\gamma' = \gamma_0 + E_{Bulk} + E_{Strain}$$

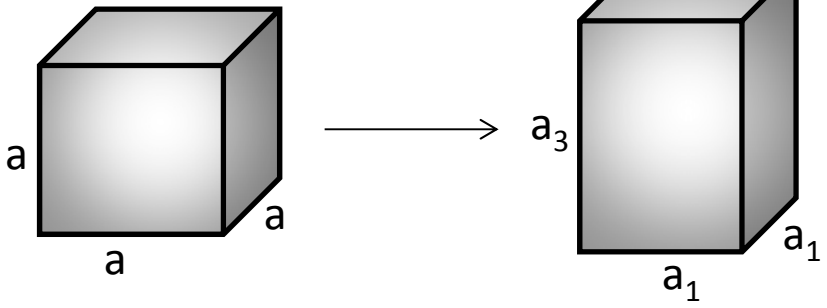
Physical foundations of material Science – G. Gottstein

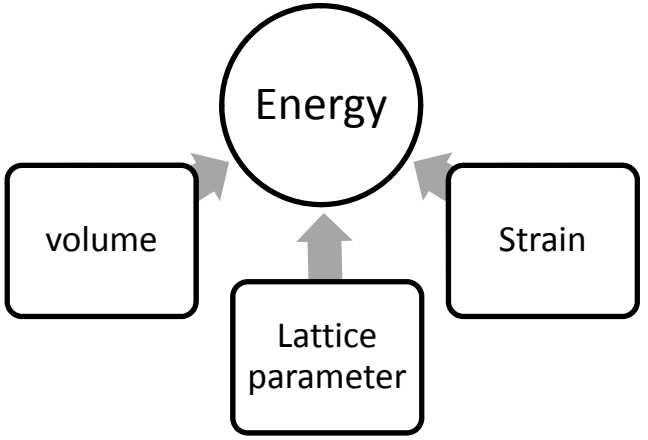
Bulk study and their results

Systems engaged:

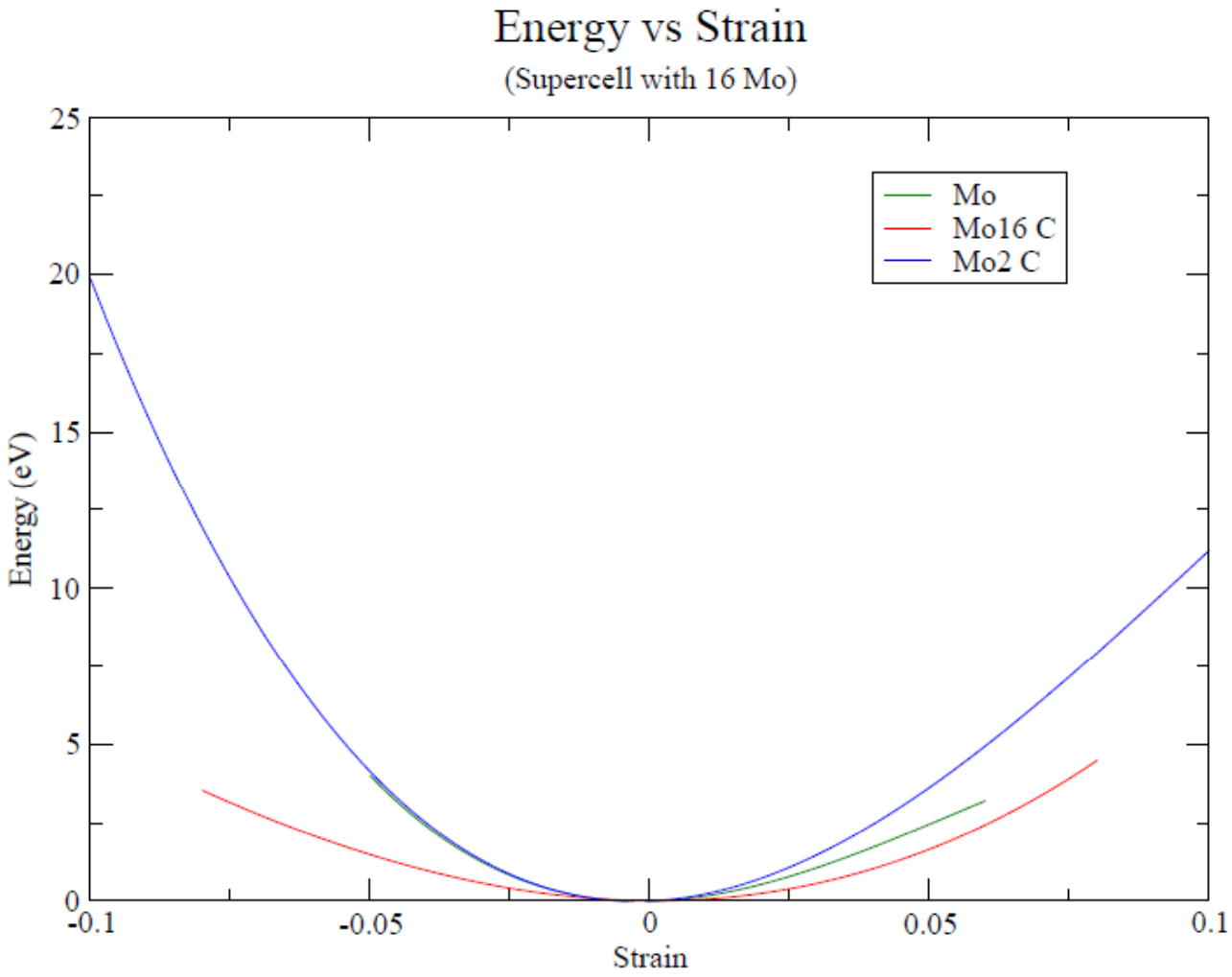
- Mo
- $Mo_{16}C$
- $Mo_{16}C_8$

Biaxial strain:

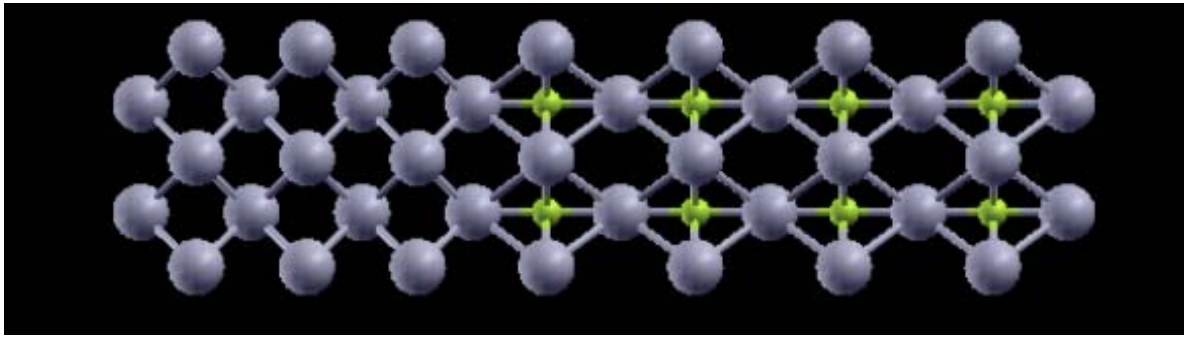


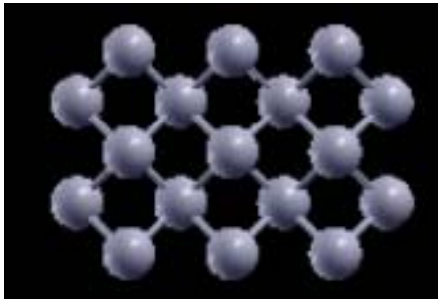


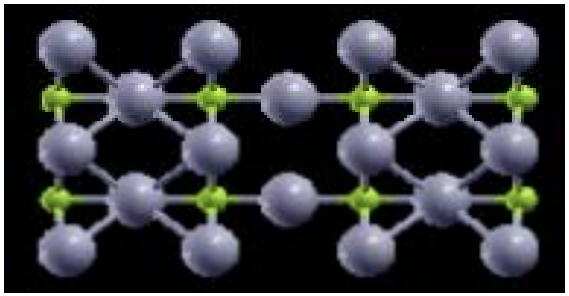
Bulk study and their results



Coherent interface







$\gamma = (E_{Tot} - E_{Bulk}) / 2A$ (Interface energy)

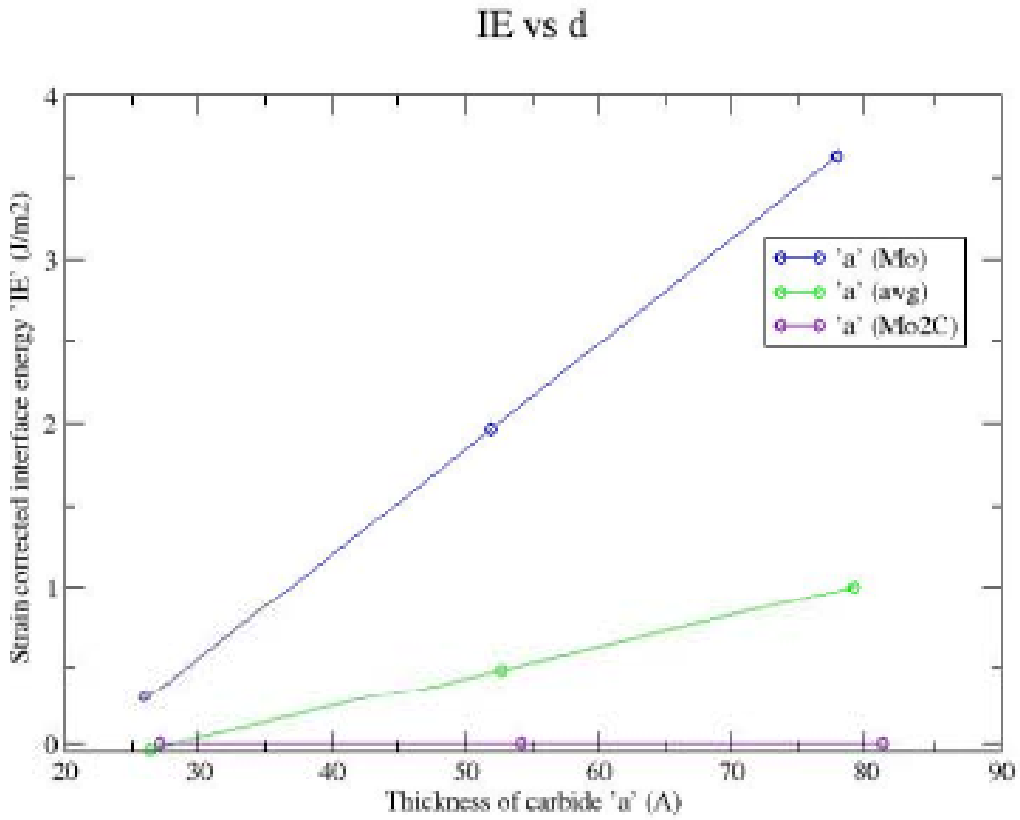
$W_{sep} = [E_{FS} - E_{Tot}] / 2A$ (Work of seperation)

$\gamma' = (\gamma_0 + nE_{Mo2C} + mE_{Mo} + n\varepsilon_{Mo2C} + m\varepsilon_{Mo})/2A$ (Strain corrected interface energy)

$\gamma_0 = \gamma'(n=14, m=4) - \gamma$ (Constant)

Interface study and results – Mo||Mo_2C

Lattice constant(Å)	W_{sep} (J/m2)	γ (J/m2)
3.0712 (avg)	**4.424**	**0.544**
3.1520 (Mo)	3.274	0.705
2.9907 (Mo_2 C)	4.063	0.828

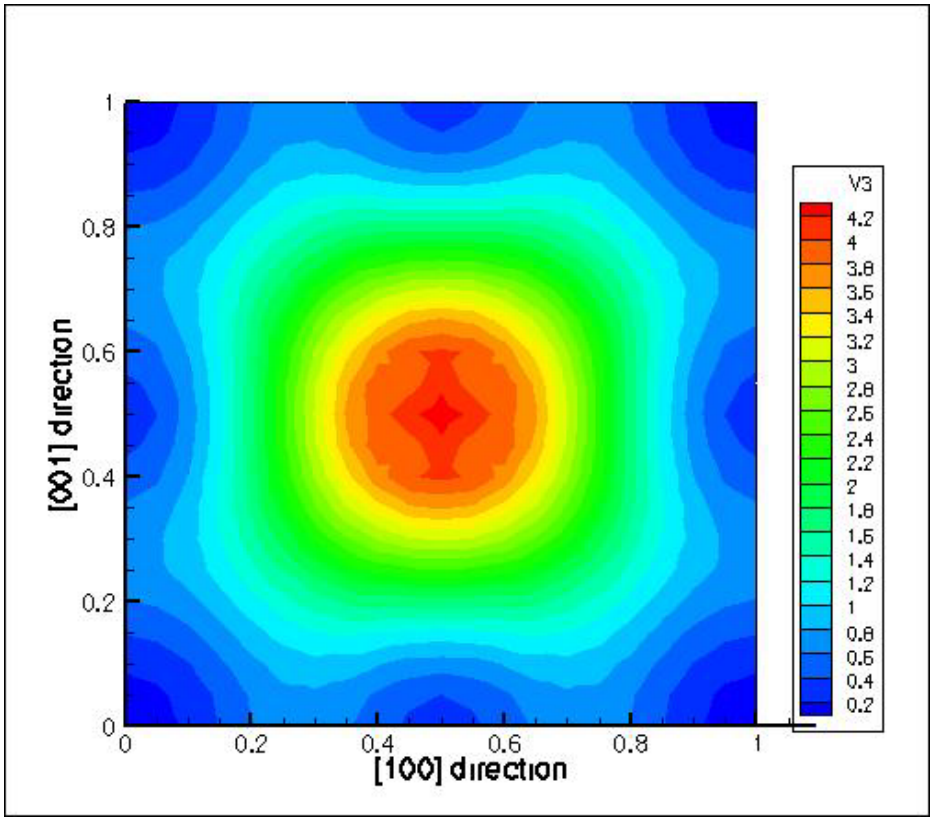


Interface study and results – Mo||Mo_2C

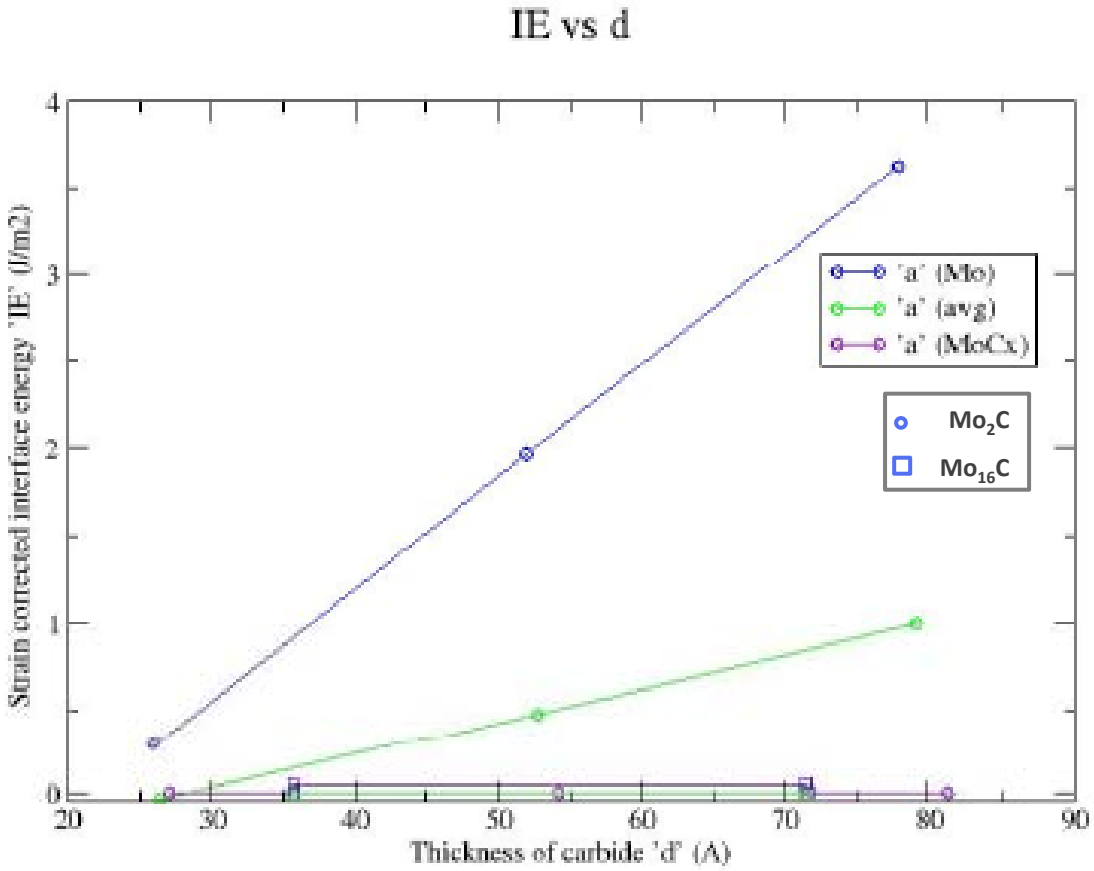
Gamma surface study

b = 1/2[100]

= 1/2[010]



Interface study and combined results



Conclusions

- Bulk system
  - Energy accompanying the strain for Mo and carbides have been calculated
- Coherent interface
  - Coherency is expected only until ~30Å thickness of carbide in the case of Mo||Mo_2C
  - Coherent interface could be observed in the case of Mo||$Mo_{16}C$ due to the lower carbon concentration
- The semi-coherent interface has to be modeled

Acknowledgements

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EUROPEAN UNION
Investing in our Future
European Regional
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