I: Electronic structure calculations of ordered cubic-based Mg-Li alloys

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II: Microstructural evolution of $\alpha+\beta$

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Background

- Mg alloys have, in the past decade, received revolutionary attention which emanated from the need of lightweight materials in transportation and allied industries, wherein intrinsic strength to weight ratio is of paramount importance.
- Al, Li, Zn, Mn, etc., identified as suitable main alloying elements candidates.
- Due to atomic size, mobility, solute solubility.
- Due to their properties, with lightness and recycleability in the forefront, they are potential candidates to replace steel and aluminium alloys in many structural and mechanical applications.
- Lithium at a density of 0.53 g/cm^3 not only enjoys superiority lightness, but also a useful phase change to bcc when alloyed at about 11wt% concentration and increase in ductility.
- High amount of experiment work been carried out on Mg-Li alloys, few investigations has been done through theoretical *ab initio* techniques.

Mg & Mg alloys: Properties

Advantages

- Availability (8th most abundant 2.7% earth crust)
- Extremely light
- High strength:weight ratio
- Excellent machinability
- Good castability
- Inherent recyclability
- High dumping capacity
- Good creep resistance

Disadvantages

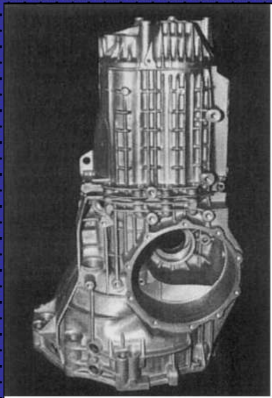
- High cost
- Poor wear & corrosion resistance
- Low elastic modulus
- Limited cold workability
- High chemical reactivity
- Limited strength at elevated T

Need: Weight reduction in transport without sacrificing structural strength

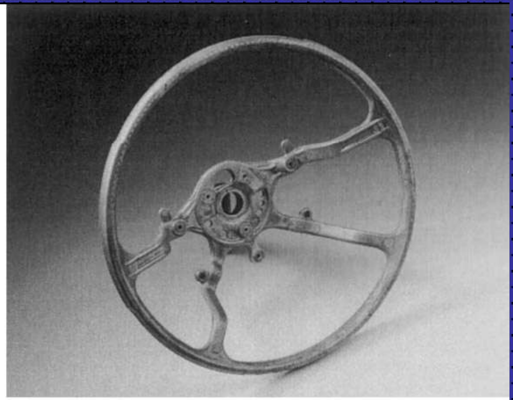
Applications: automotive & aerospace components, computer parts, mobile phones, sporting goods, handheld tools, household equipments

Other possible Appl. : implants due to low weight & inherent biocompatibility

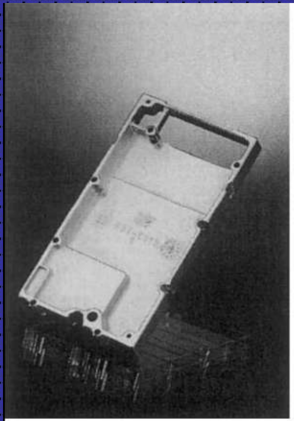
Applications



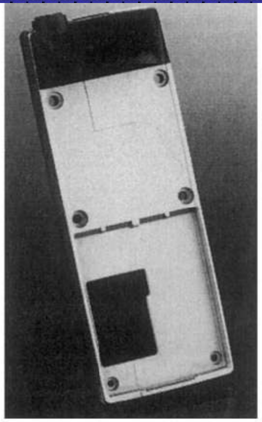
Gear Box Housing



Steering Wheel Frame

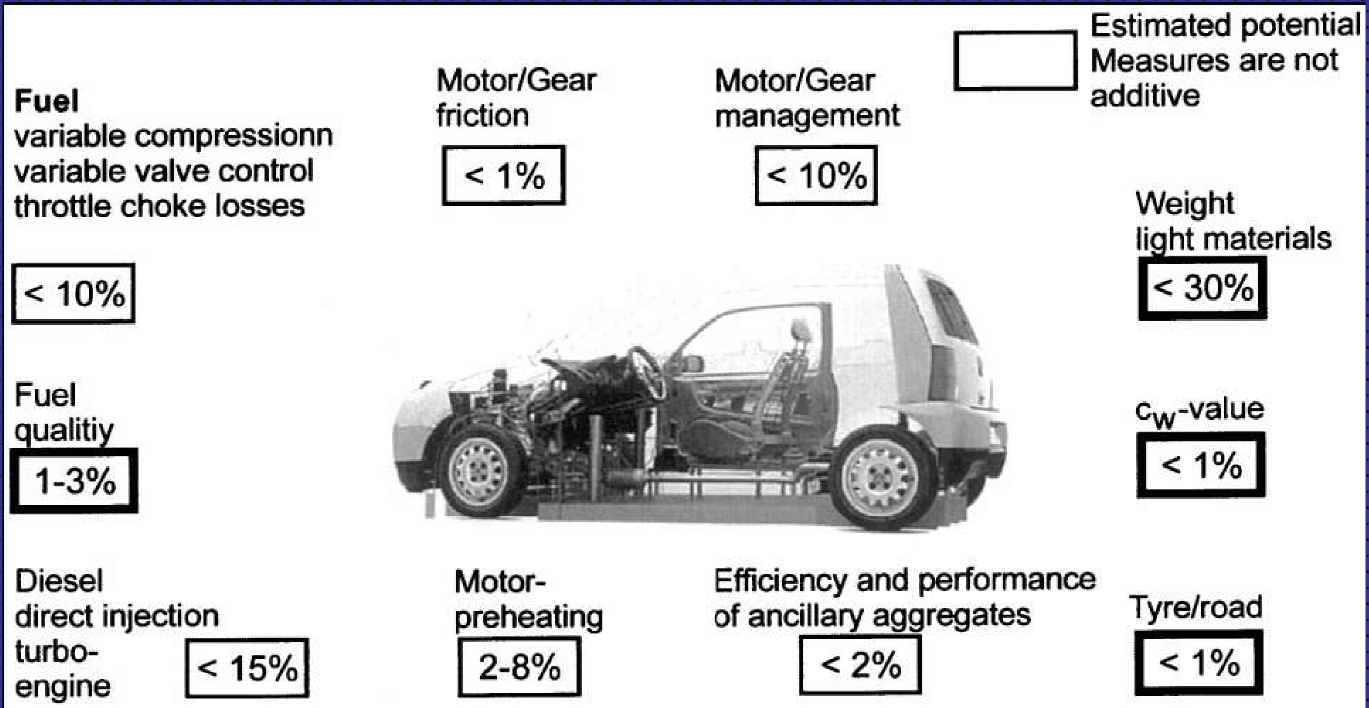


Screen Housing

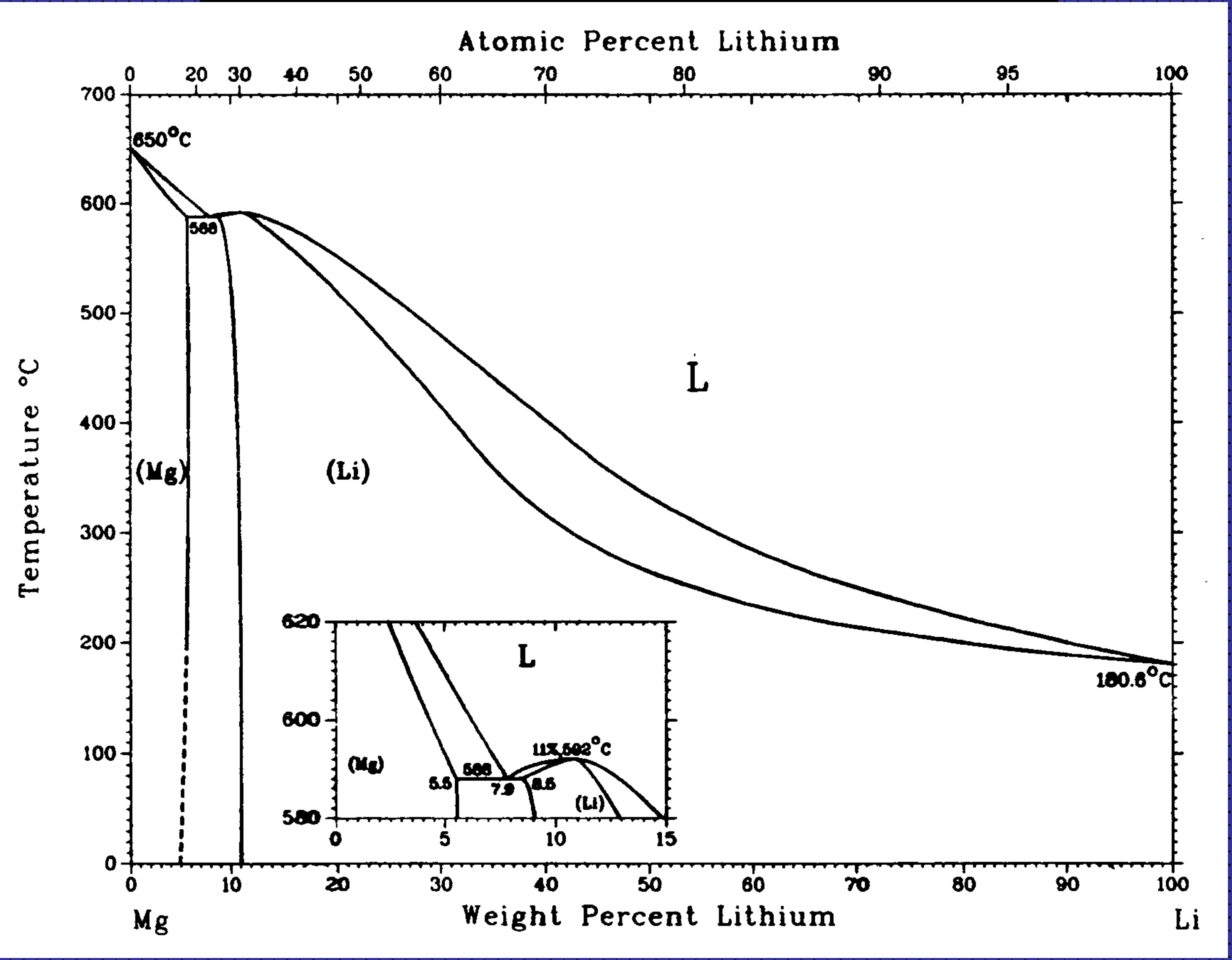


Units For Mobile Handset

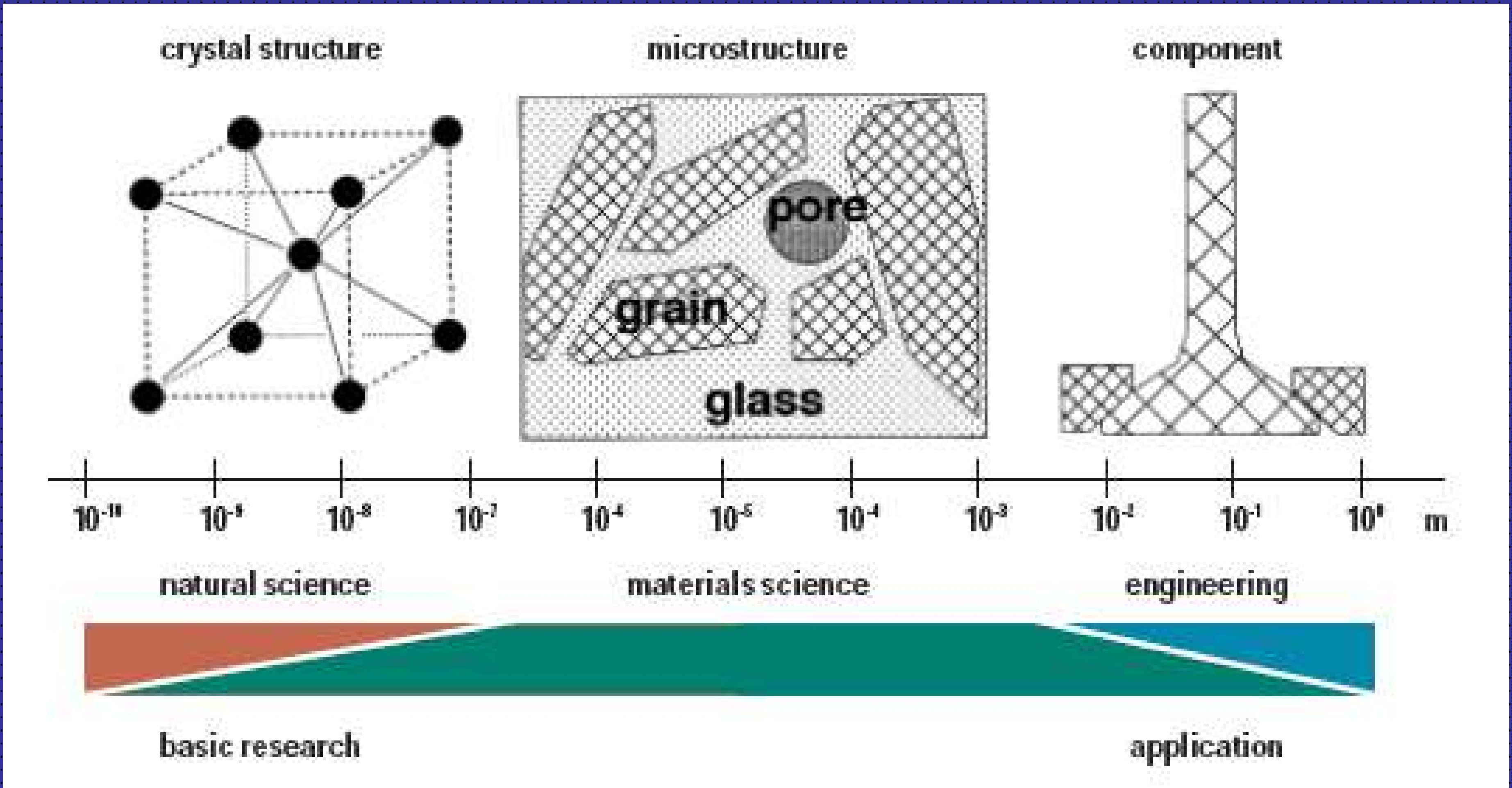
Mordike et al



Mg-Li Phase diagram



Hierarchies of length scales

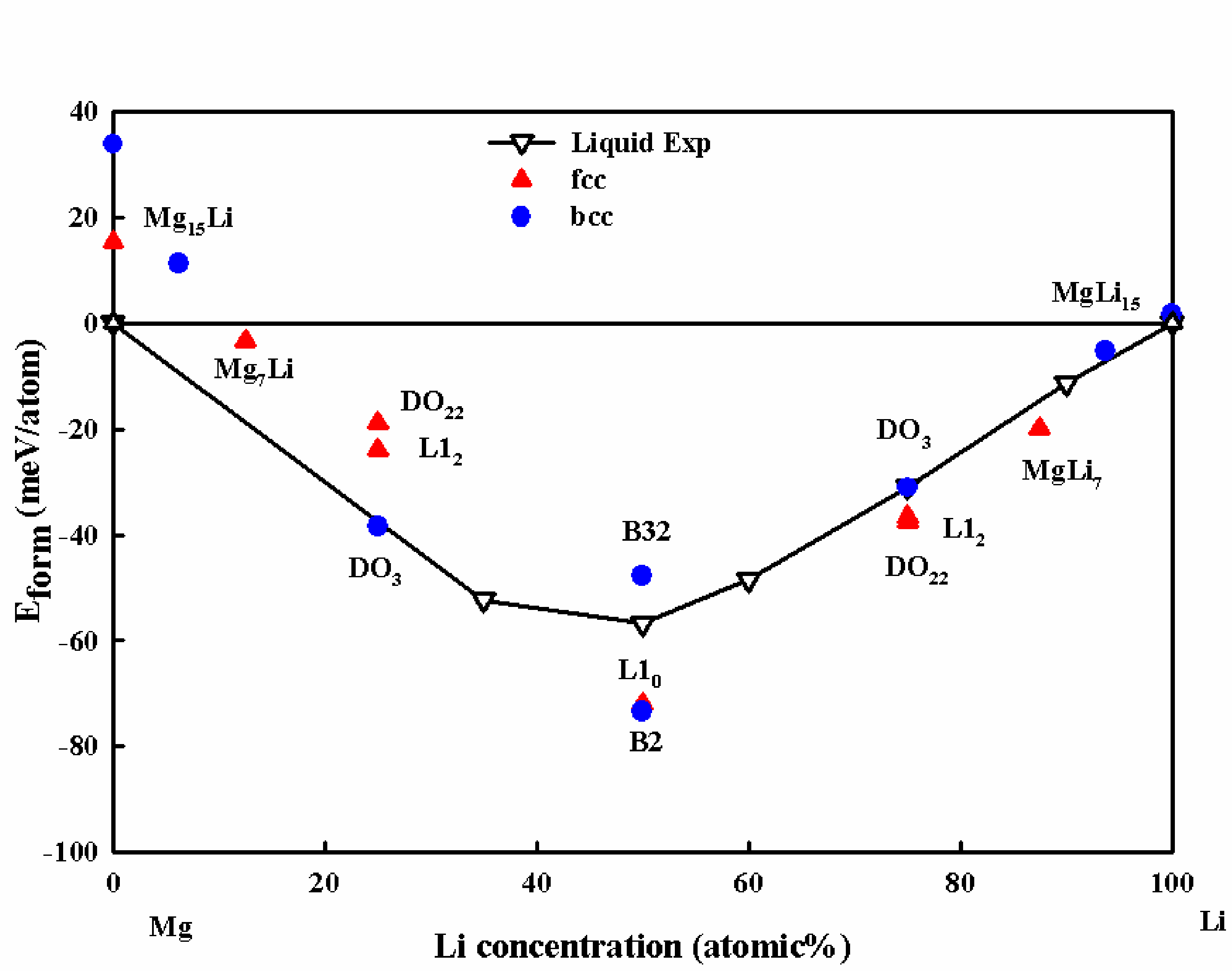


I:Methodology

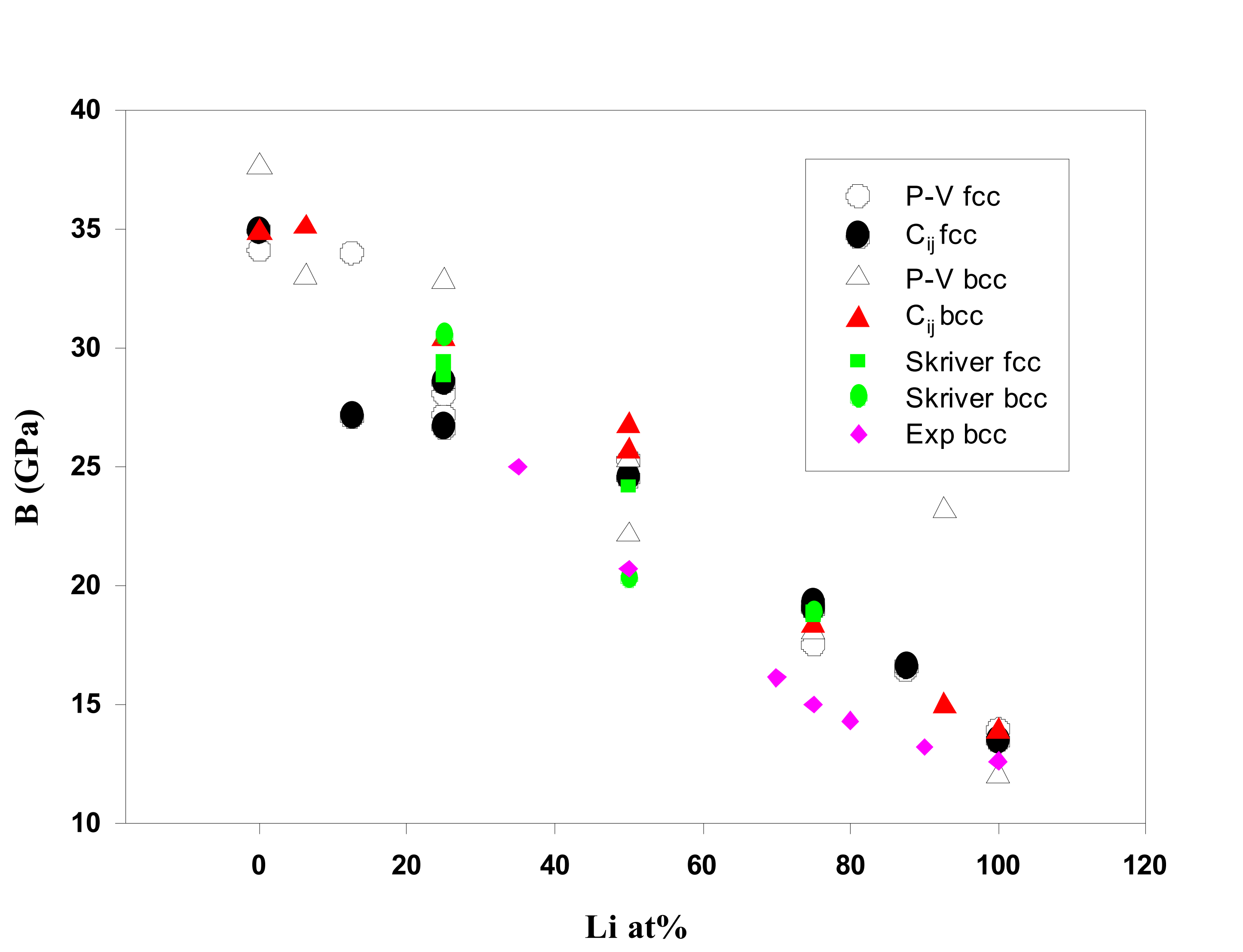
- Total energy code, CASTEP, based on DFT within GGA-PBE.
- Vanderbilt ultrasoft pseudopotentials -using plane wave
- Monkhorst-Pack scheme
- Energy cut-off & k-points were converged

Results

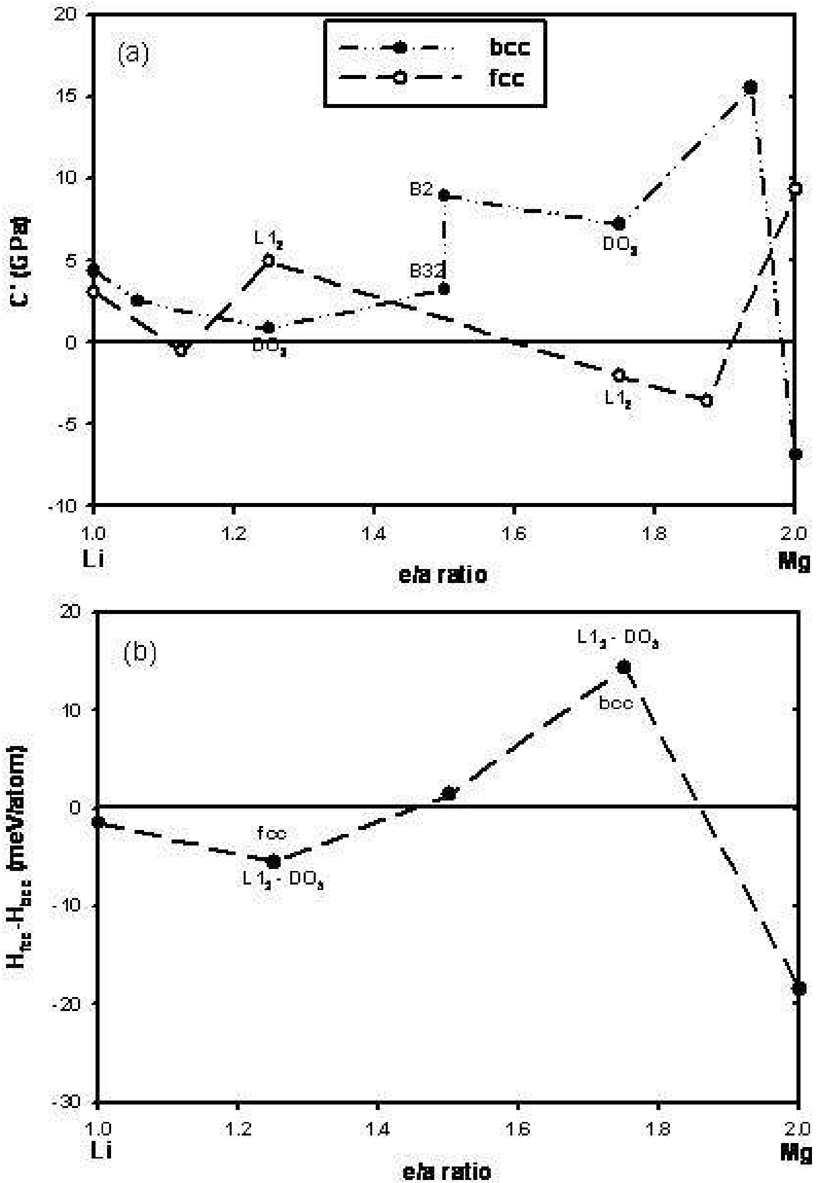
Heats of formation

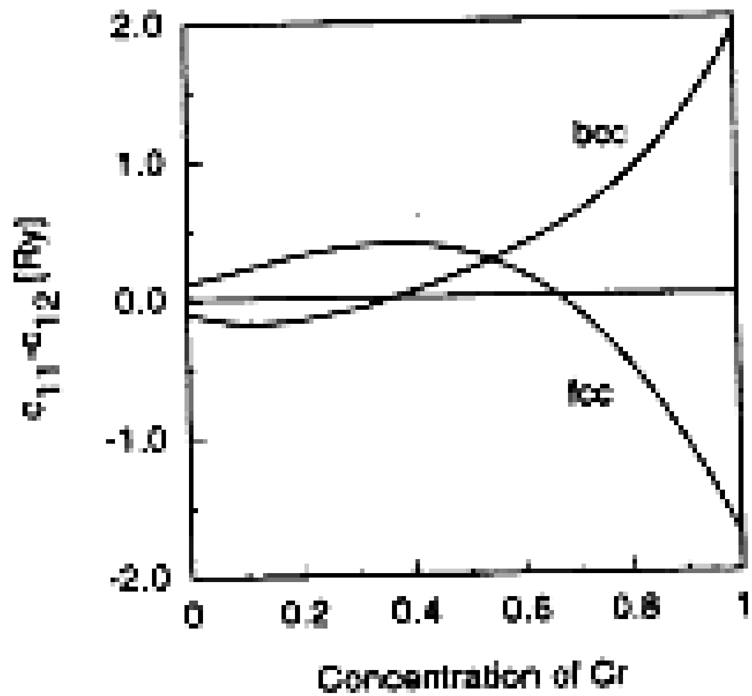


Bulk Modulus



Shear, Energy correlation





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Conclusion

- Bulk moduli decrease monotonically with increase in Li concentration.

- Predicted heats of formation for all the different ground state superstructures result in a representative stability profile, which shows that the DO_3, B2 and DO_{22} structures are the most stable amongst various phases having Mg_3Li, MgLi and $MgLi_3$ compositions, respectively. The similar stability is also being investigated by the use of density of states (DOS).

- Stability profile hcp-bcc-fcc-hcp is predicted

- Elasticity studies predicts stability of DO_3 structure in the $\alpha + \beta$ region

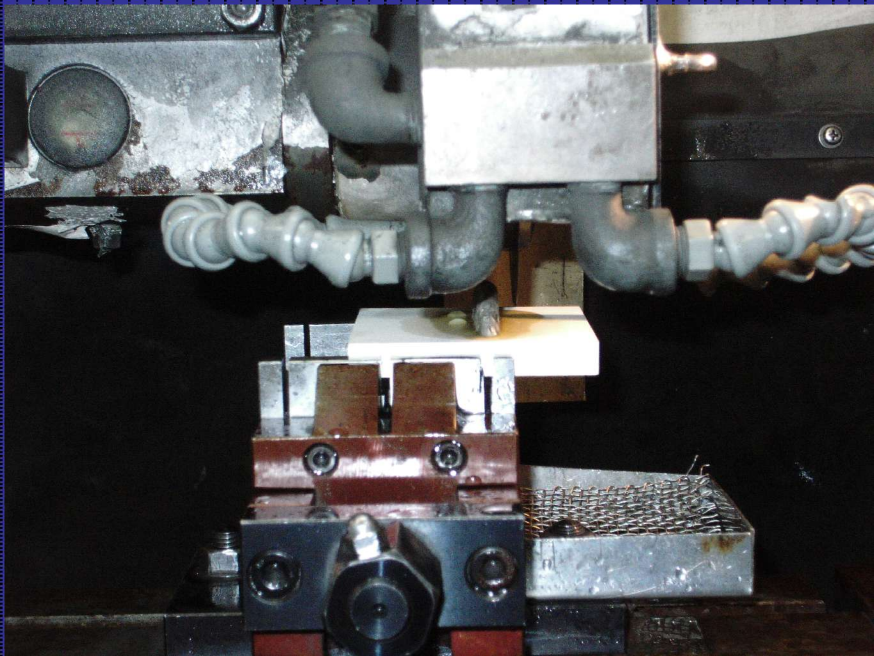
- Correlation *C' vs e/a* & *ΔE vs e/a*, region where bcc is very stable compared to fcc, the shear modulus is positive for bcc but negative for fcc (i.e. the fcc lattice is the mechanically unstable) and vice versa.

II: Microstructural evolution of $\alpha+\beta$ region of MgLi alloys

- From ab initio predictions, exp. were conducted as follows
  - Preparations of Mg-Li samples
  - Heat treatments
  - Microstructural phase observations
  - Mechanical tests
  - Structure evolution (OOFEM)

Sample Preparation Conditions

- Arc Melting furnace
- Argon - protecting atmosphere



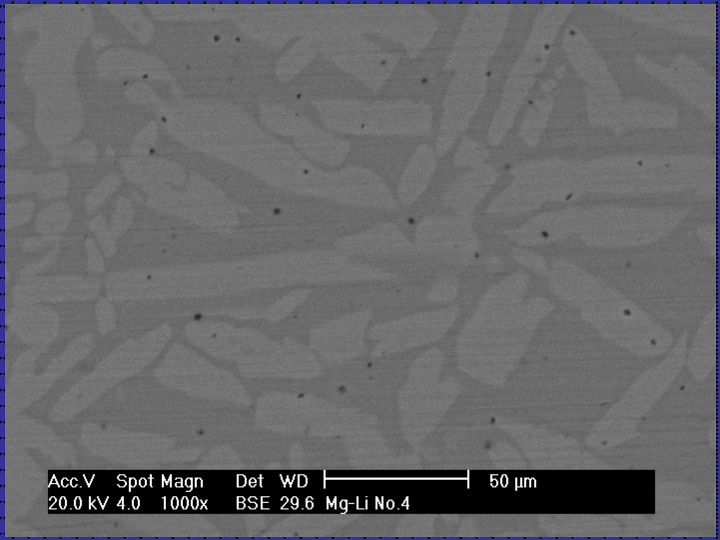
Composition of samples

Sample	Li content (wt.%)	Relative ρ g/cm^3
Mg-9Li	8.69	1.44
Mg-10Li	10.03	1.40
Mg-11Li	10.99	1.37
Mg-12Li	12.01	1.35

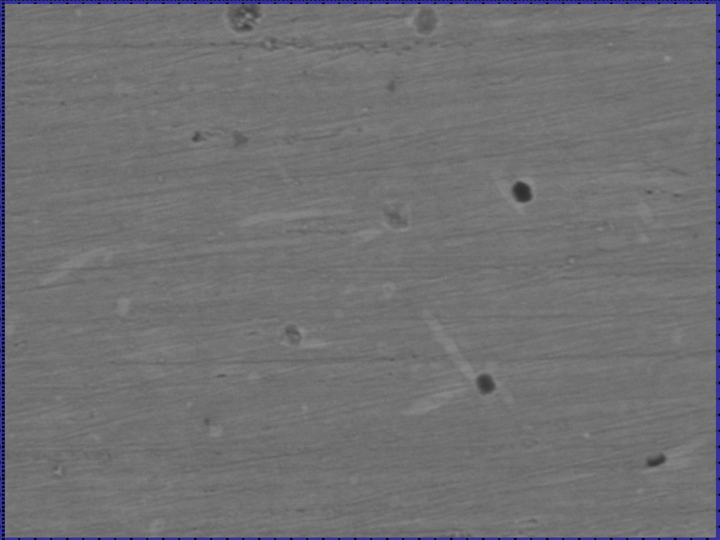
SEM

PHILIPS XL 30, Au coater

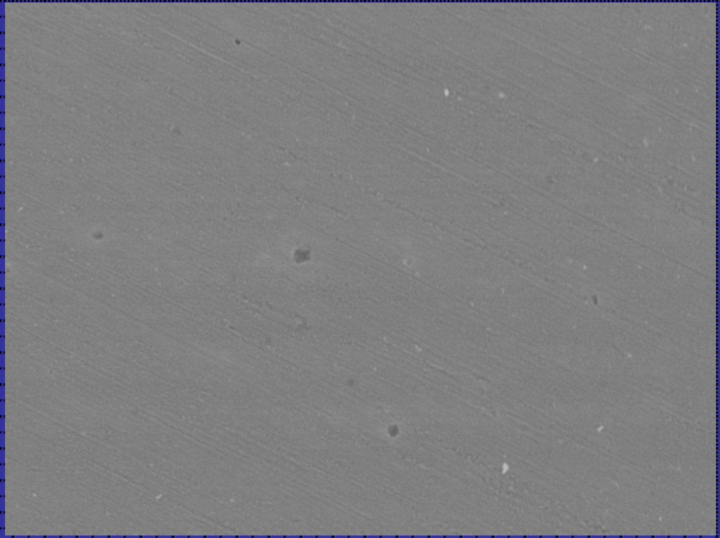
SEM Observations:RT



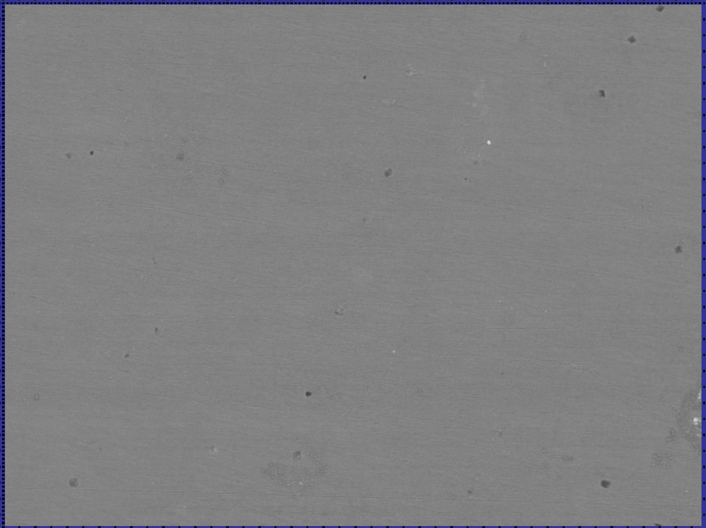
(a) Mg-9Li alloy



(b) Mg-10Li alloy



(c) Mg-11Li alloy



(d) Mg-12Li alloy

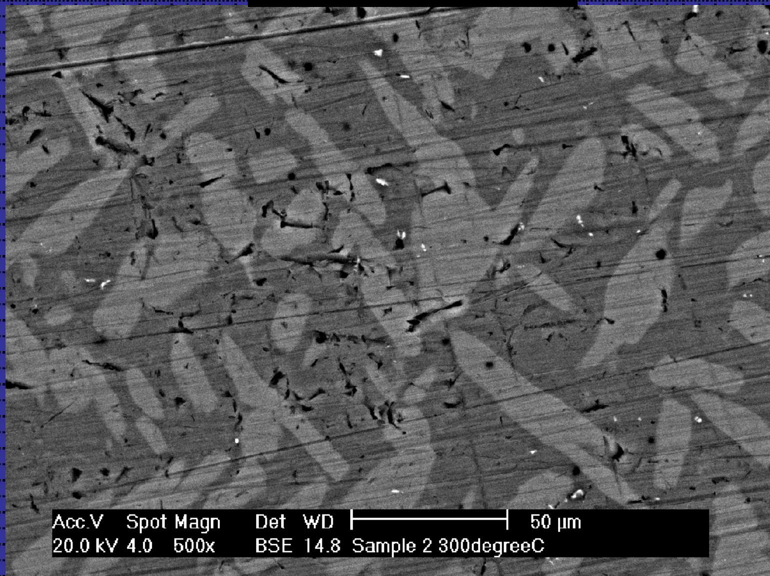
Microstructure Analysis

Sample	Phases present	Observation
Mg-9Li	α+β (hcp+bcc)	Evenly distributed dual phase alloy
Mg-10Li	α+β (hcp+bcc)	Dominant β phase with α precipitates
Mg-11Li	β (bcc)	Single phase with slight oxidation
Mg-12Li	β (bcc)	Single phase

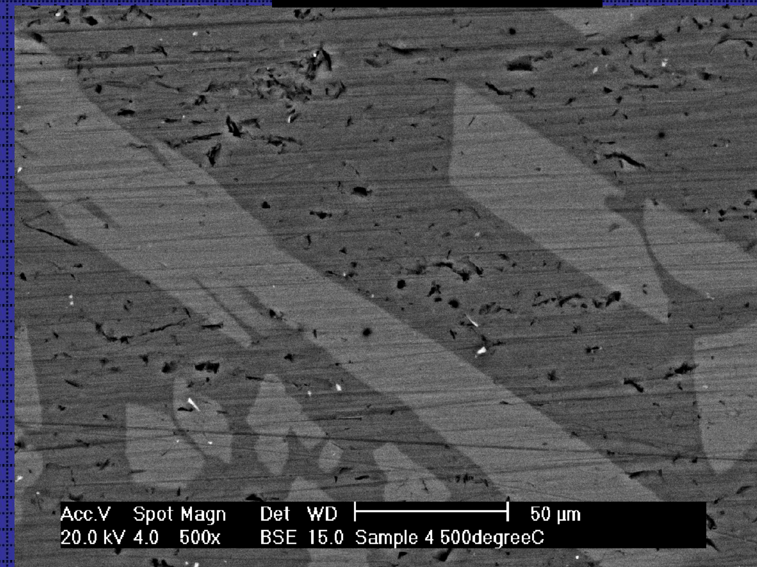
Heat treatments

Heat treatment Results

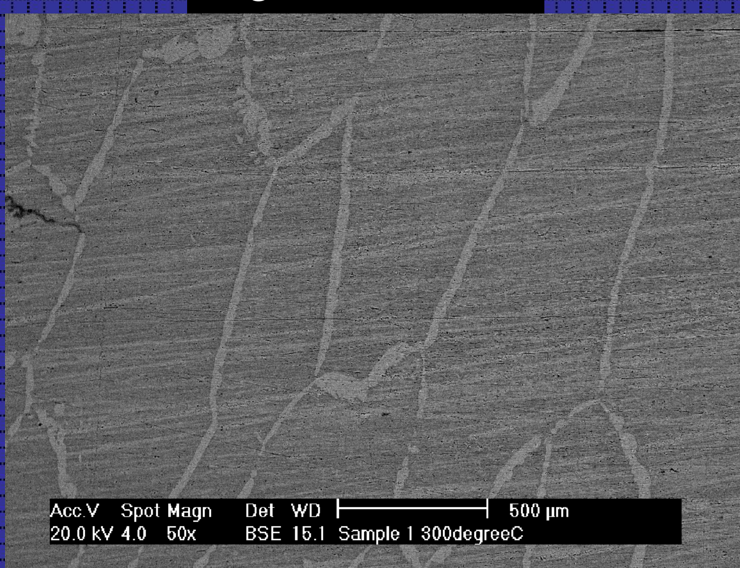
Mg9Li 300 °C



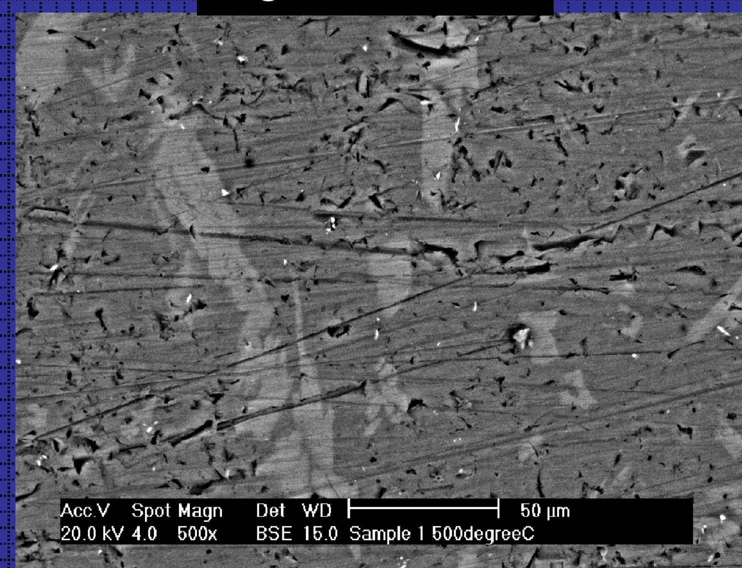
Mg9Li 500 °C



Mg10Li 300 °C

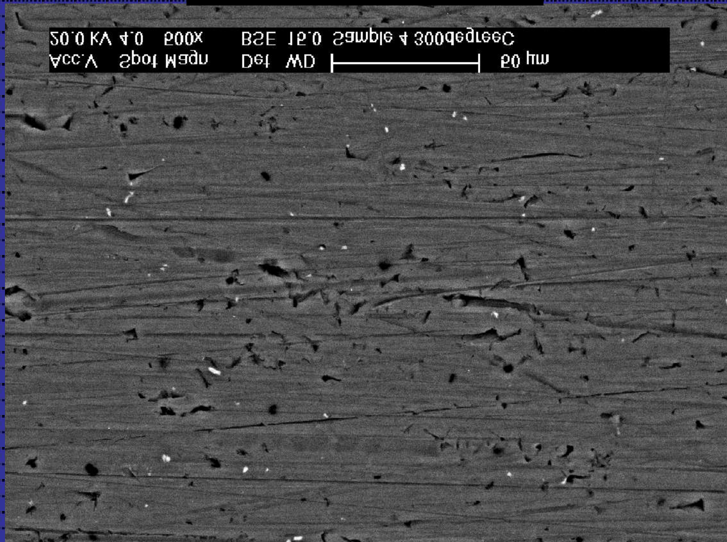


Mg10Li 500 °C

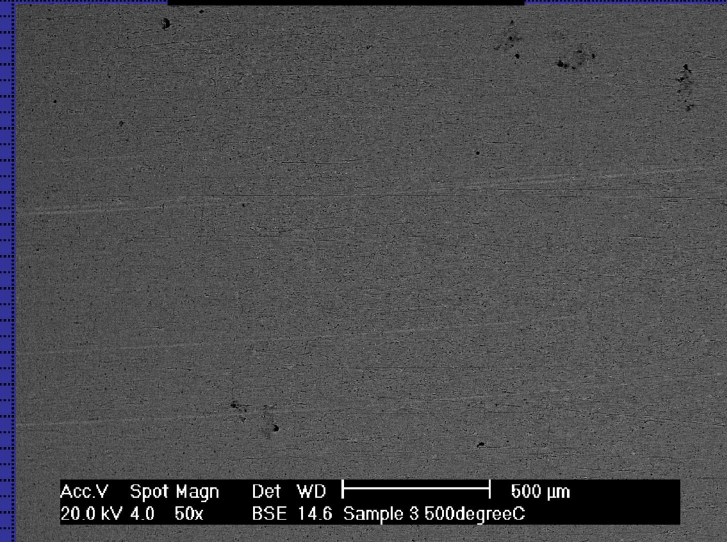


Heat treatment Results

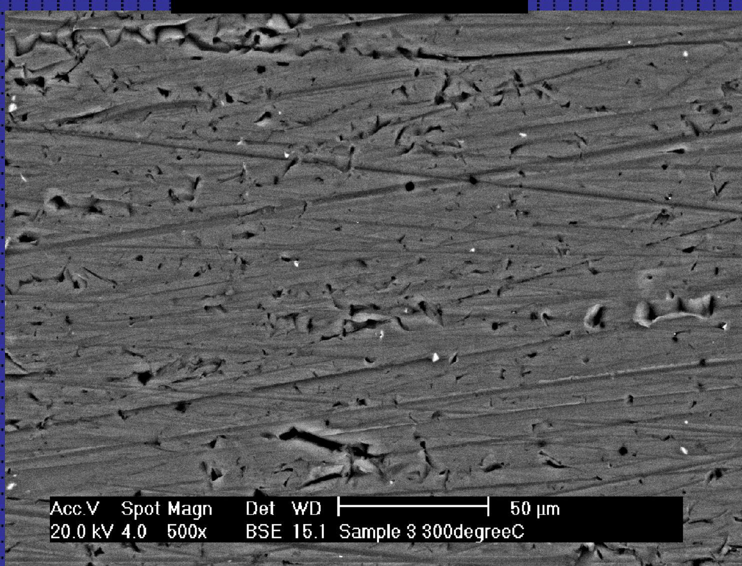
Mg11Li 300 °C



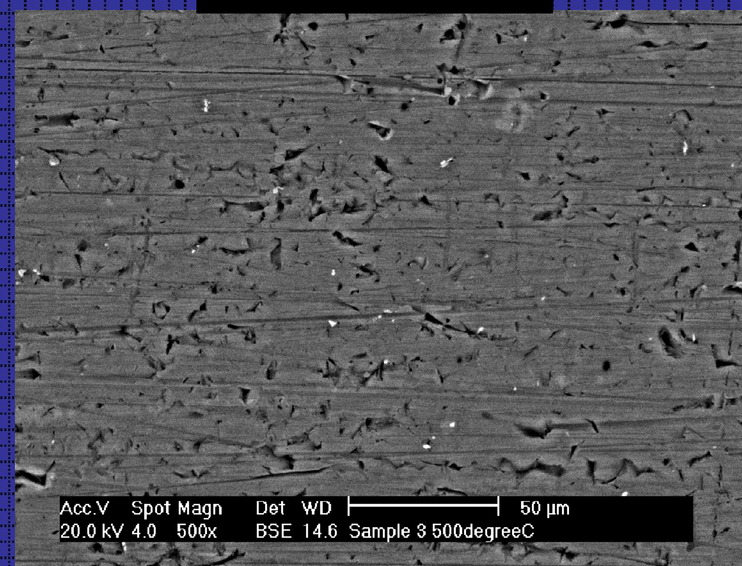
Mg11Li 500 °C



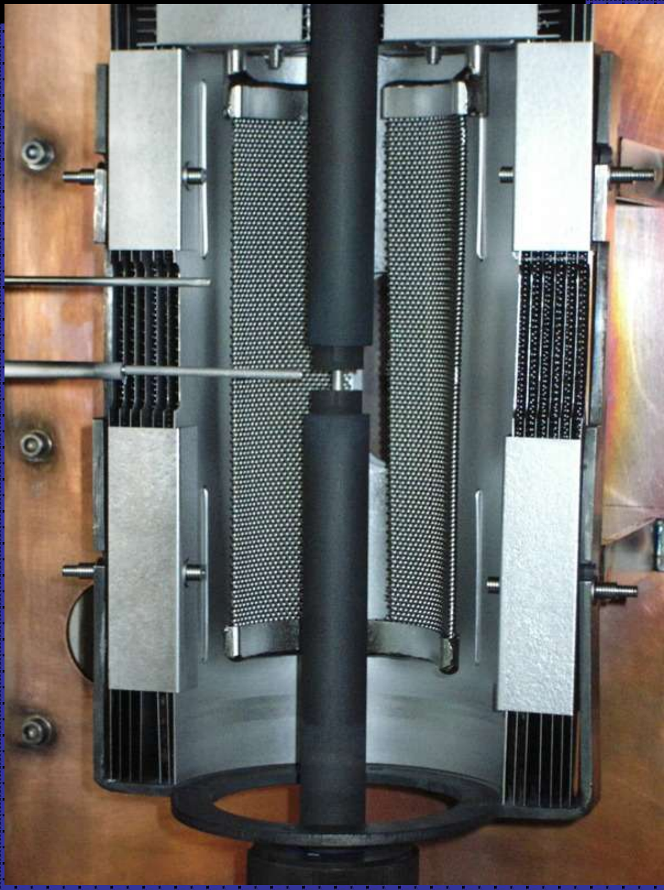
Mg12Li 300 °C



Mg12Li 500 °C

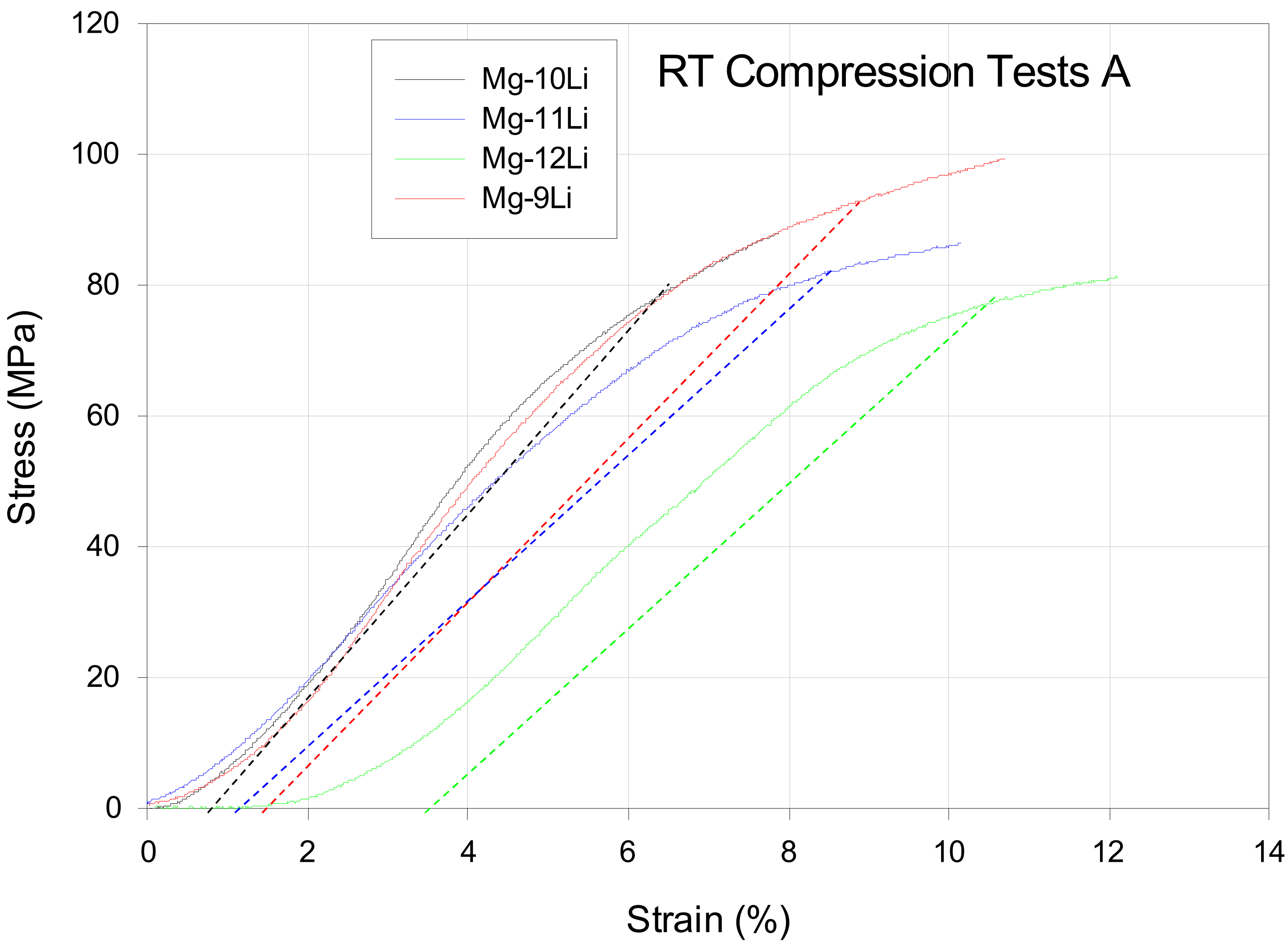


Compression Tests



Instron machine – cylindrical specimens
d=3.87 mm   *l*=6.80 mm
Compression/deformation speed = 0.001 mm/s

Compression Tests



III: Future work - Bridging length-scales

Multiscale Materials Design

Ab initio Calculations (CASTEP, VASP)

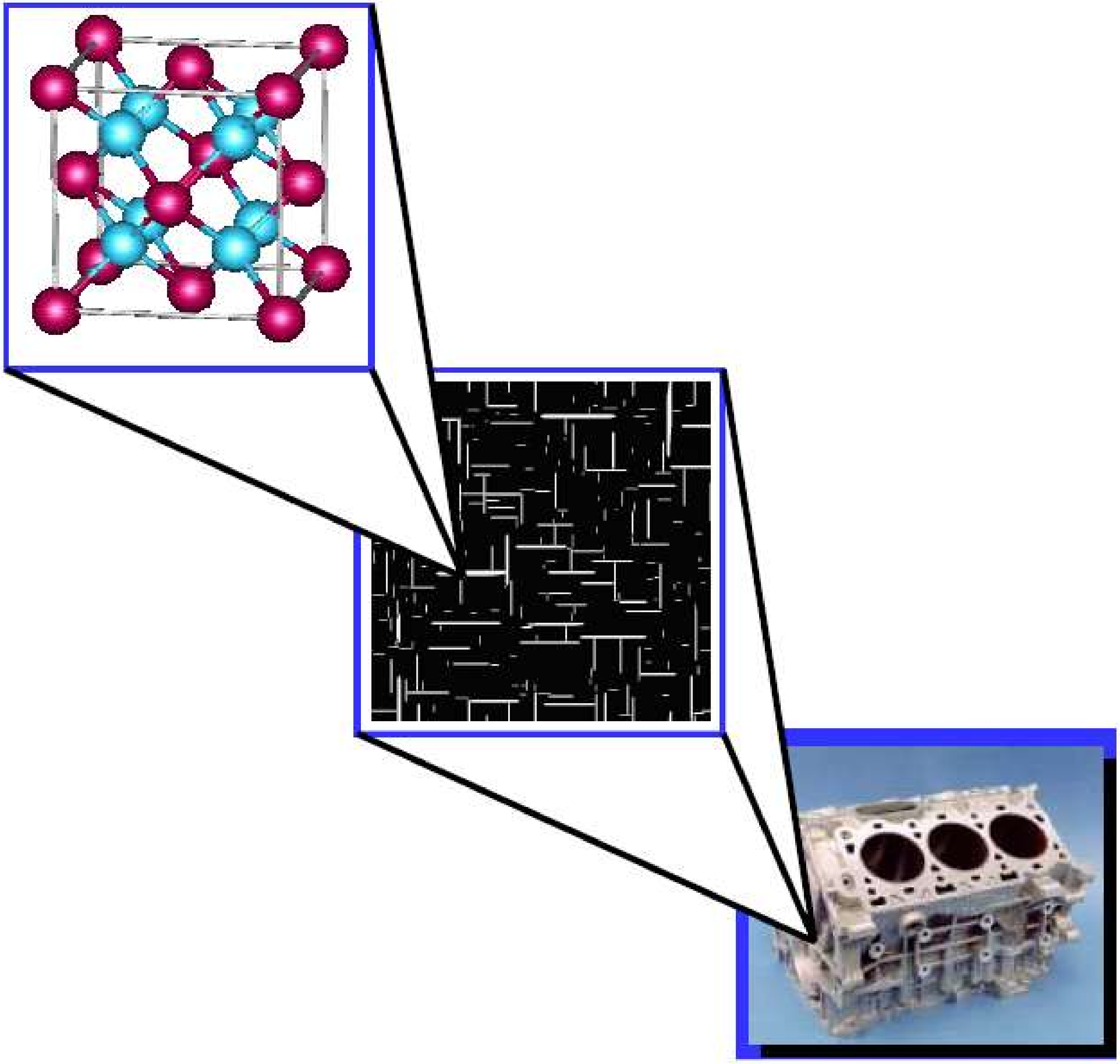
Thermodynamic Calculations (CALPHAD, Thermo-Calc)

Phase-field Model (Microstructure)

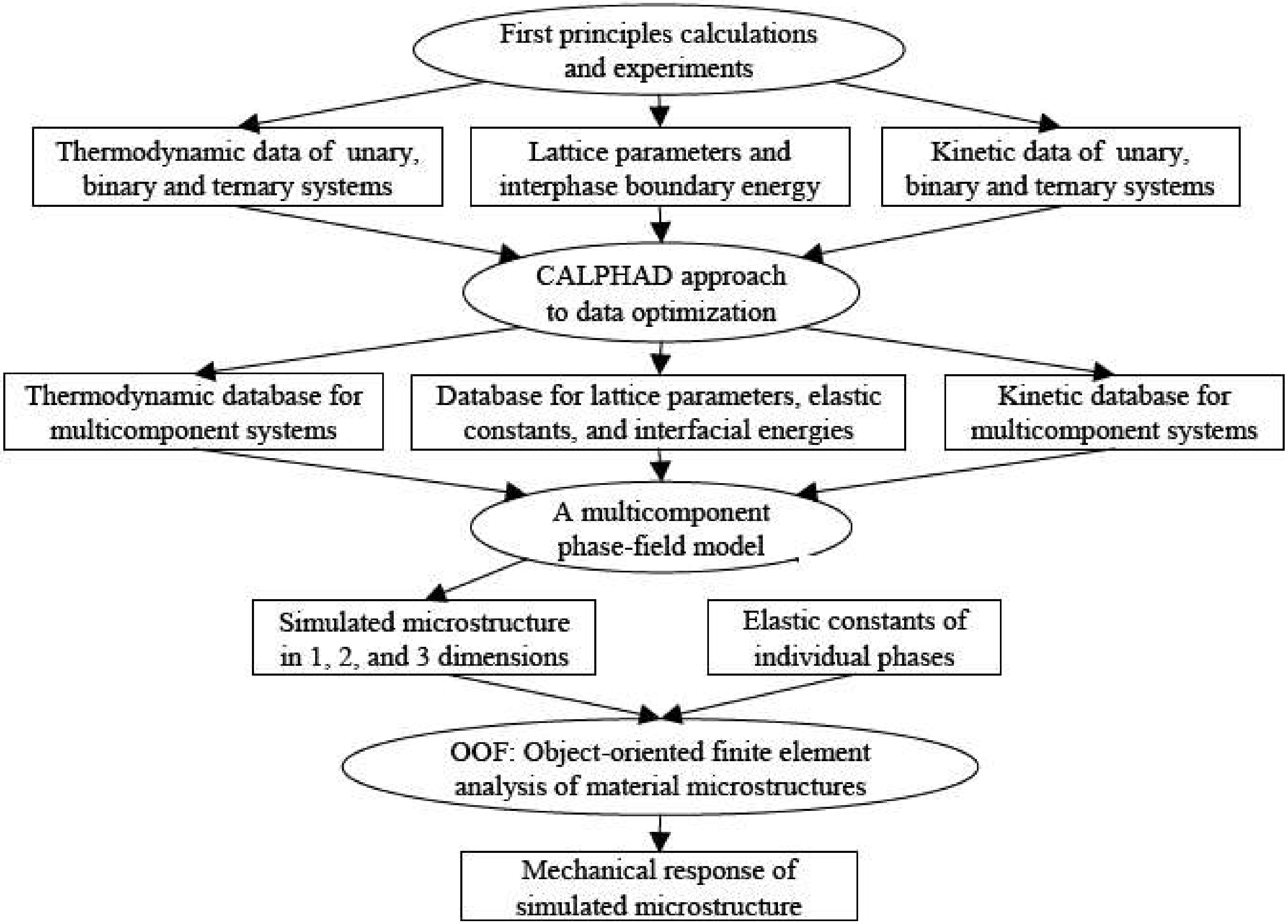
Microstructure Evolution (OOF)

- **Binaries Mg-X (X = Al, Zn, Si,)**
- **Ternaries MgLi-X (X = Al, Zn, Cd, Ti, Ca, Pb, Mn)**
  MgZn-X, MgAl-X (X = Li, Zn, Cd, Ti, Mn, RE)
- **Solid phase transformation**
  Phase diagram predictions

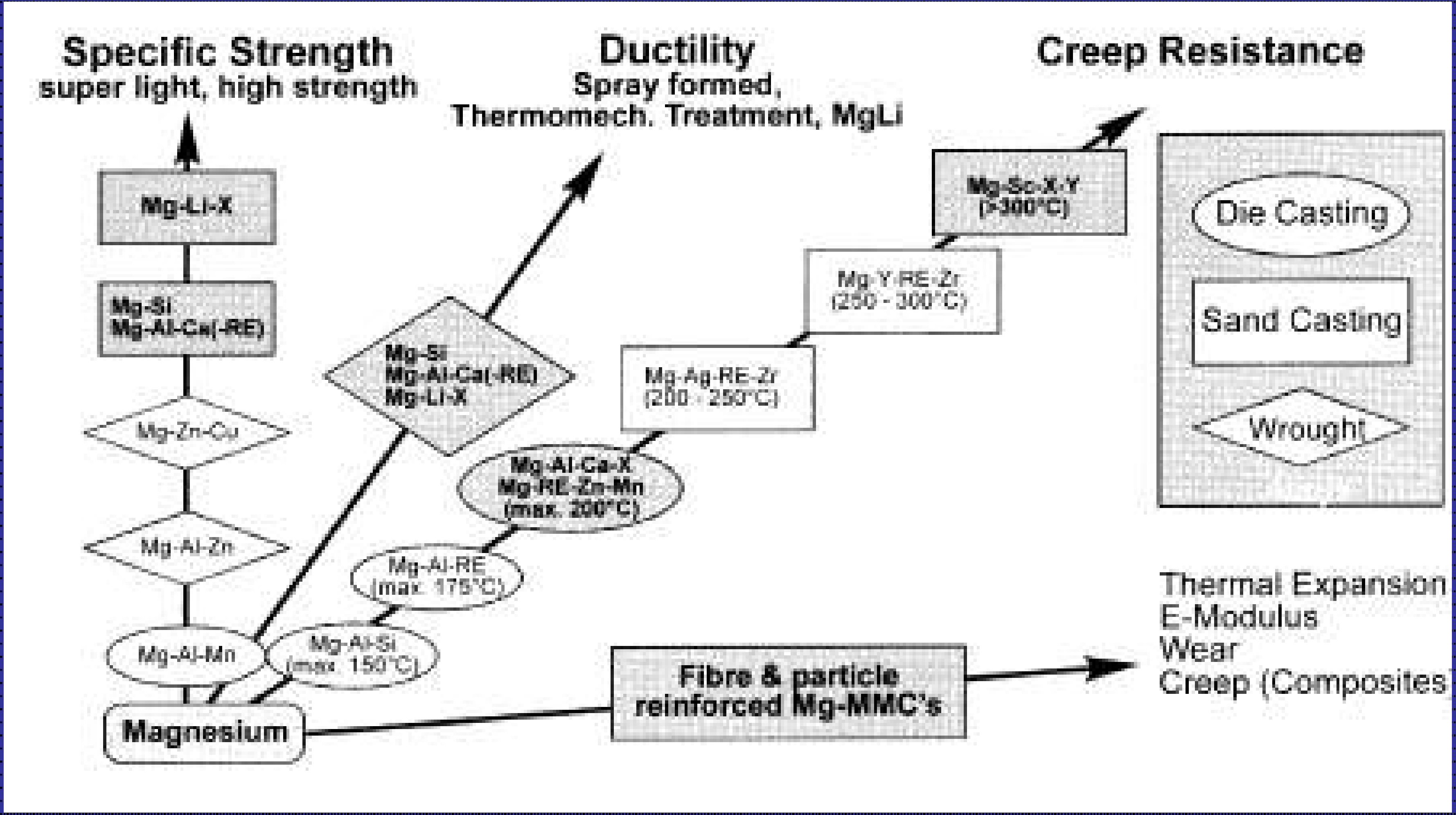
Multiscale Material Design



Integrated set of Comp tools for Multicomponent Materials Design



Directions of Mg alloy development



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  - MMC
  - NIMS
  - CSIR