DOE Program Merit Review Meeting
Southern Regional Center for Lightweight Innovative Design (SRCLID)

Advanced High Strength Steel Project

June 7-11, 2010

Prime Recipient: Center for Advanced Vehicular Systems
Mississippi State University

Agreement Number: (# DE-FC-26-06NT42755)

MSU Principal Investigators: Mark Horstemeyer, Paul Wang
DOE EE Manager: Carol Schutte, William Joost
NETL Program Manager: Magda Rivera

Project ID LM018

Materials Design of Steel Alloys

Researchers: Seong-Gon Kim, Hongjoo Rhee, Sungho Kim, Mark F. Horstemeyer

Goal: Design a new high-strength steel alloy with improved strength and ductility for automotive applications.

Objectives: (1) Identify the fundamental mechanisms at quantum mechanical and micromechanical level that determine overall strength and ductility of steel alloys. (2) Investigate the interaction among different phases of high-strength steel alloys. (3) Investigate the effect of micro-alloying elements to the material properties of high-strength steel alloys. (4) Investigate the effect of various strengthening mechanisms to the material properties of high-strength steel alloys.

Approach:

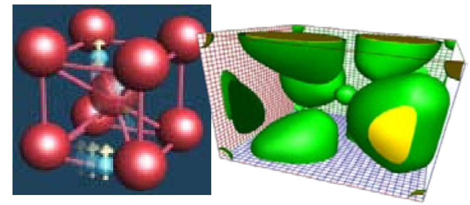
-Use a **hierarchical multi-scale methodology** to investigate the effect of precipitates and additives to the overall strength and ductility in steel alloy design for automotive applications.

-Critical issues being addressed include: selection of key micro-alloying elements, interaction of precipitate and matrix phases, and ultimately composition-structure-property relationship.

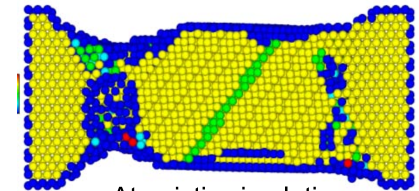
-**Quantum mechanical first-principles simulations** based on Density Functional Theory (DFT) will be performed.

-Accurate atomistic simulations will be performed using Modified Embedded Atom Method (MEAM) and force-matching-embedded-atom-method (FMEAM) potentials.

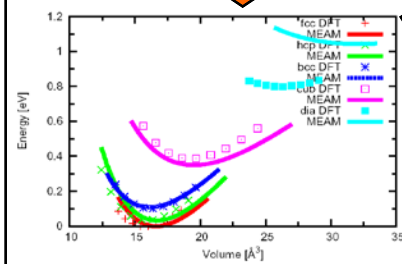
-**Large scale atomistic simulations** will be conducted to study the effect that size, shape, and volume fraction of different inclusion particles have on the material properties of steel alloys.



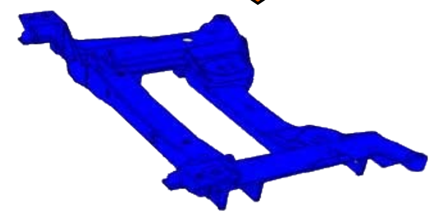
Quantum mechanical (DFT) simulations



Atomistic simulations



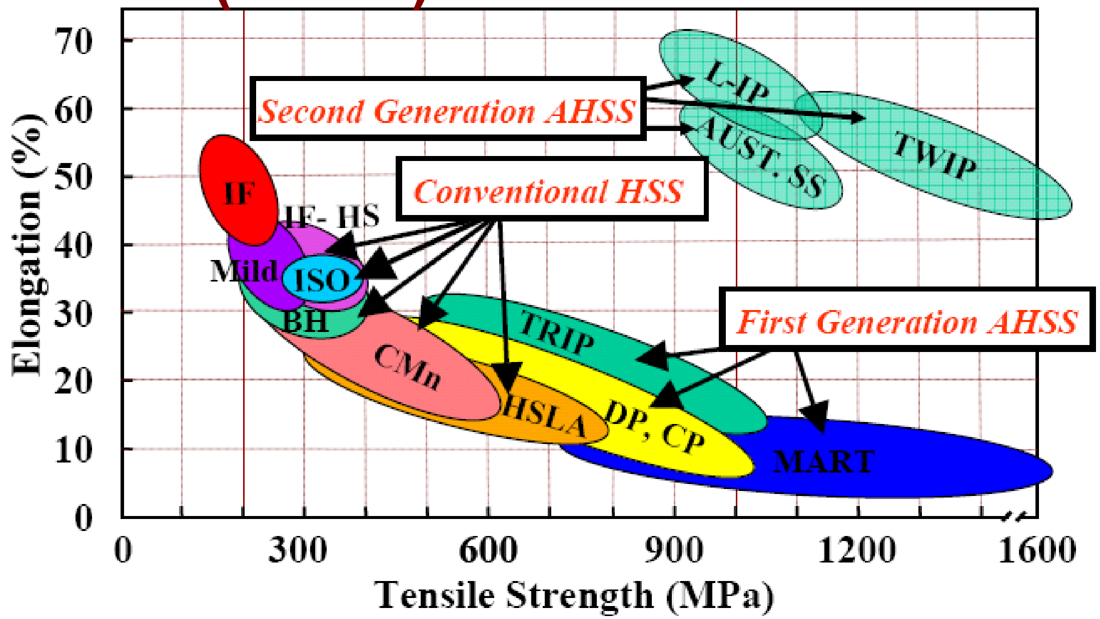
Potential construction/validation



New steel alloy design

- **Subtask 6.1** -- Construct and validate reliable inter-atomic potentials to model various phases of high-strength steel alloys
- **Subtask 6.2** -- Perform electronic and atomistic simulations to obtain the electronic, structural and mechanical properties of the main phases of steel alloys.
- **Subtask 6.3** – Perform electronic and atomistic simulations to investigate the interactions between main phases of high-strength steel alloys.
- **Subtask 6.4** – Perform electronic and atomistic simulations to investigate the effect of microalloying of high-strength steel alloys.
- **Subtask 6.5** -- Perform experiments to Investigate the effect of various strengthening mechanisms to the material properties of high-strength steel alloys.

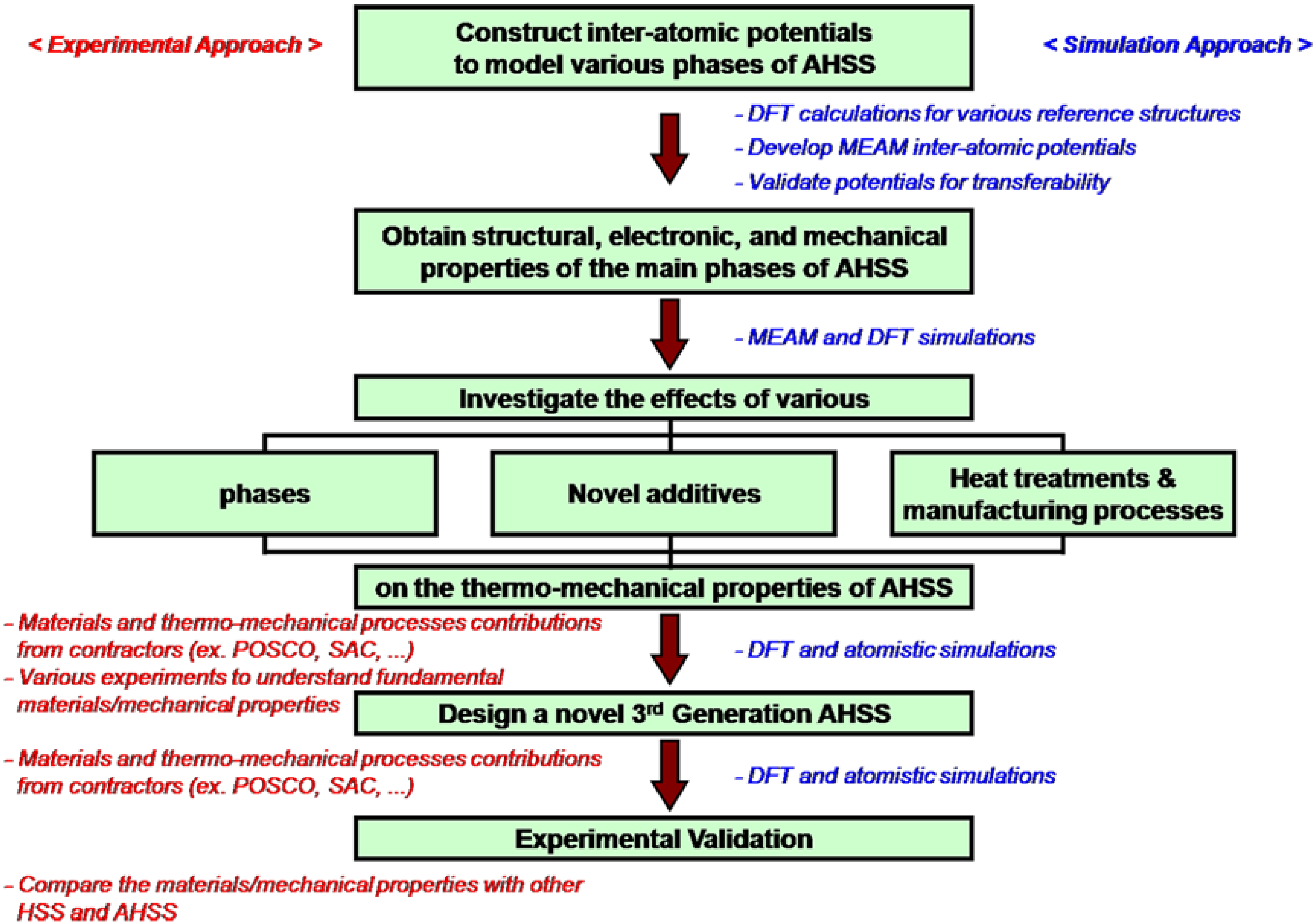
Advanced High Strength Steels (AHSS) Overview



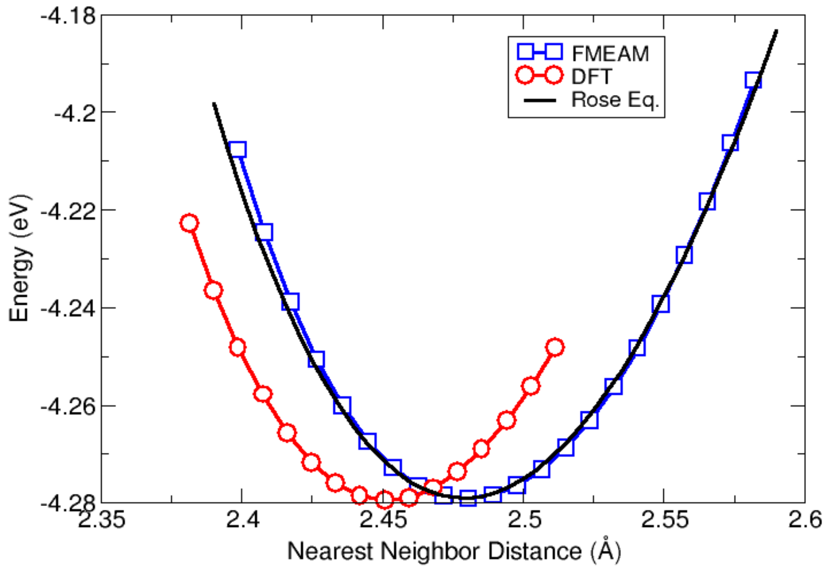
[Ref.] Advanced High Strength Steel (AHSS) Application Guidelines from www.worldautosteel.org

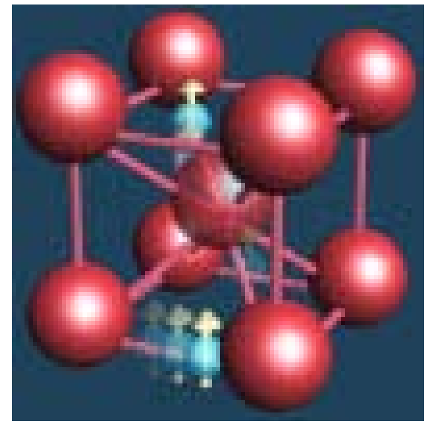
- Advanced High-Strength Steels
  - 1st Generation AHSS ⇒ need to improve formability
  - 2nd Generation AHSS ⇒ need to develop commercially available manufacturing processes
  - 3rd Generation AHSS development methodology
    - identify fundamental mechanisms at quantum mechanical and micromechanical level that determine overall strength and ductility of steel alloys
    - analyze the effect of alloy compositions and distribution of various hard phases present in steels on their thermo-mechanical properties
    - investigate the efficacy of various additives to design a novel 3rd generation AHSS alloy with improved strength and formability

Correlation with Atomistic Simulation Research

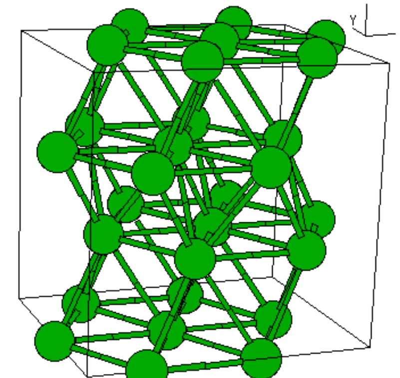


Fe Interatomic Potential

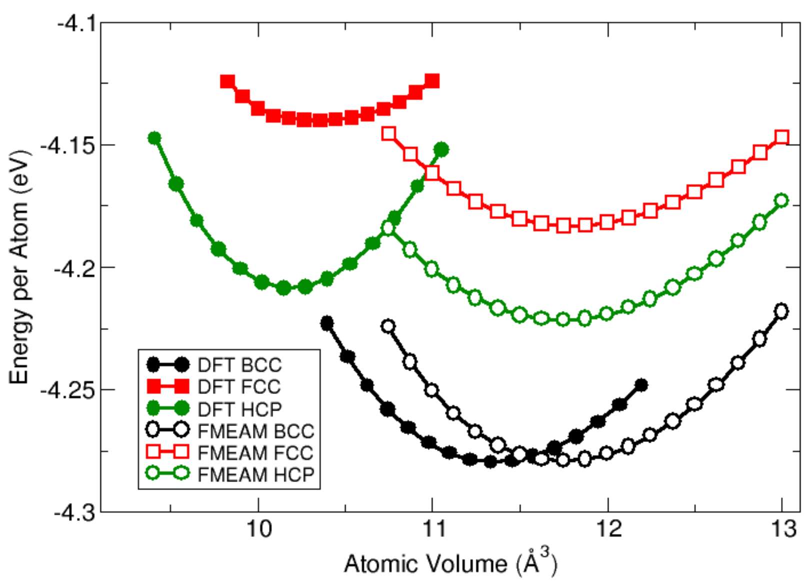


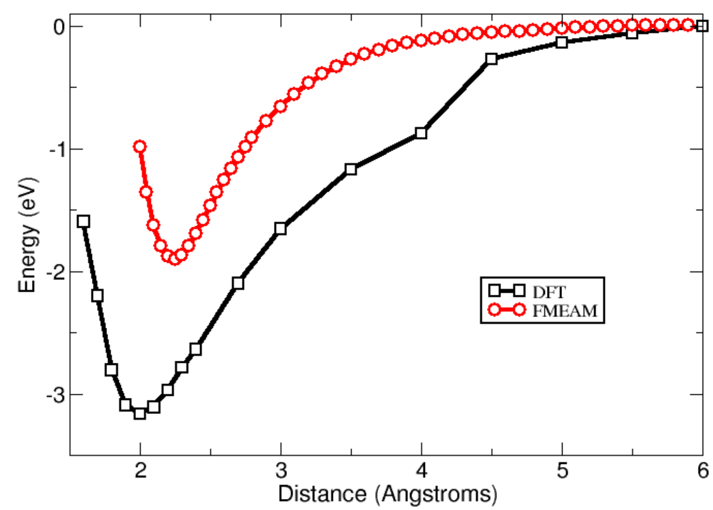


bcc Fe



hcp Fe

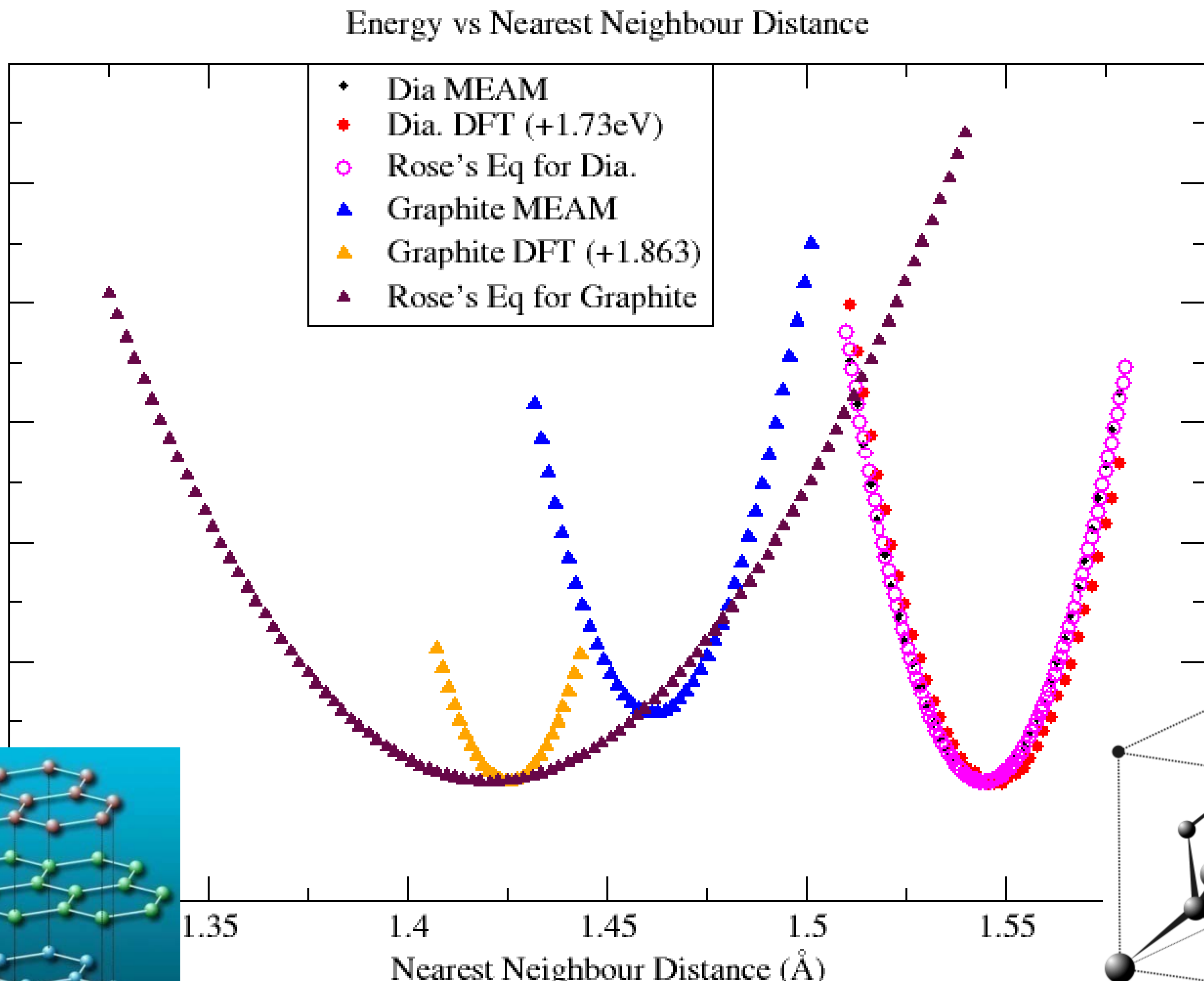


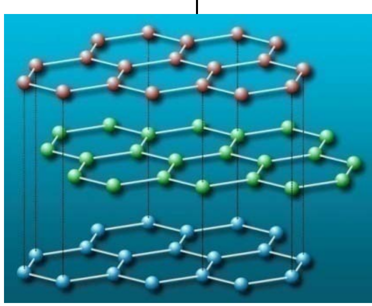


Total energy of a Fe dimer

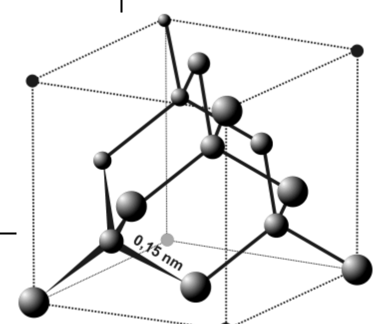
Carbon MEAM Potential

Carbon in Diamond and Graphite Structures





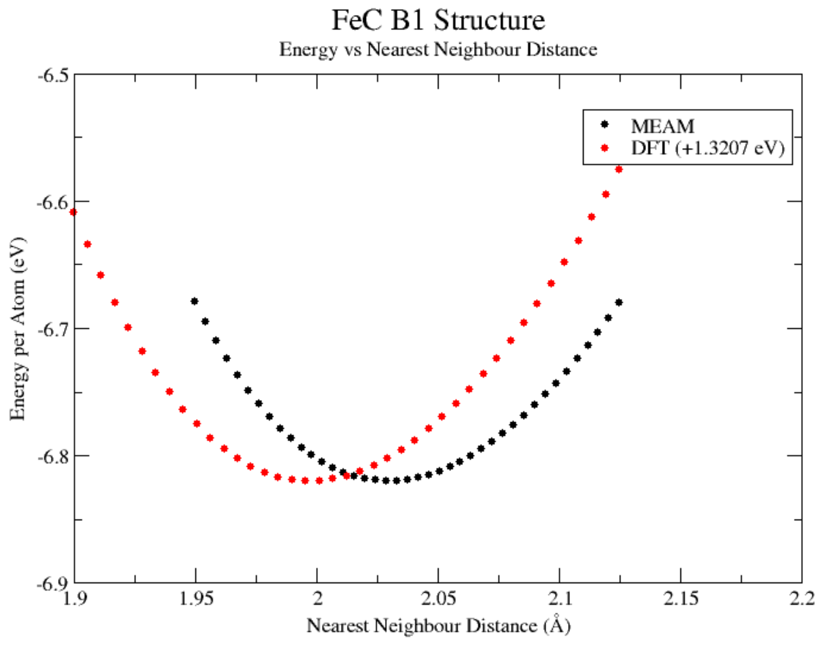
graphite

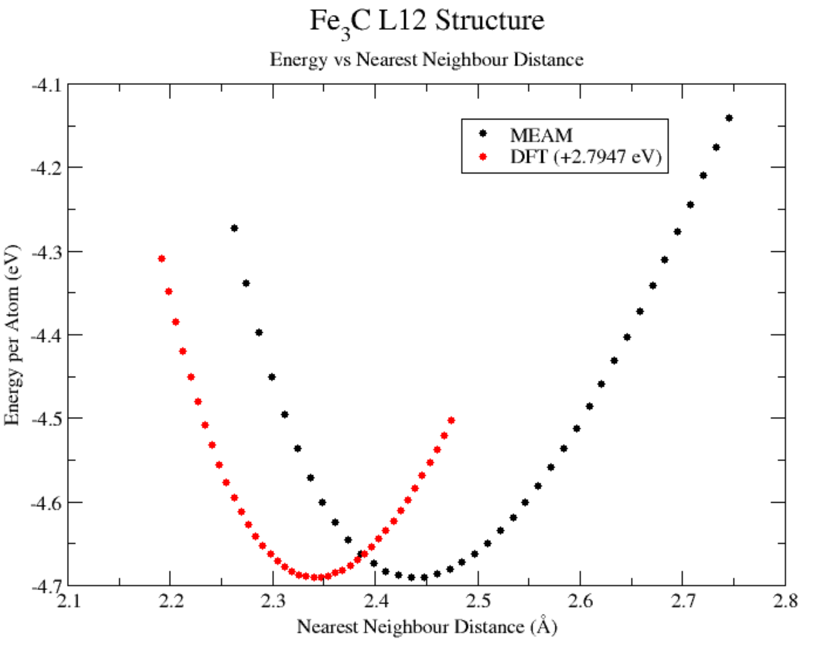


diamond

Total energy of a C dimer

Fe-C MEAM Potential



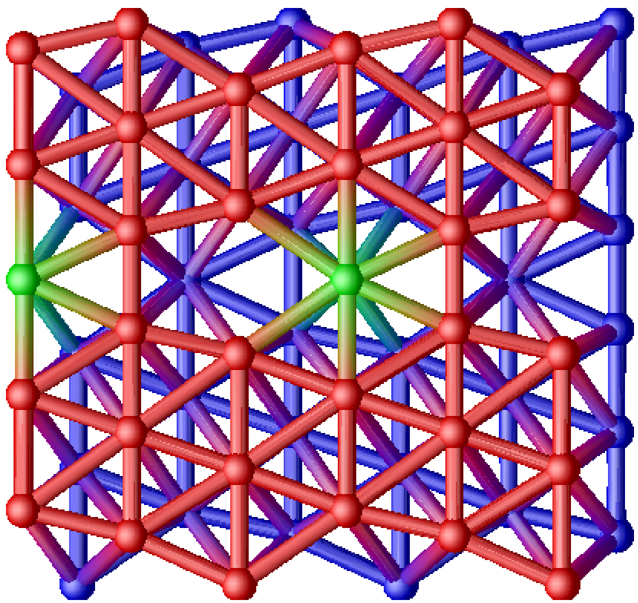


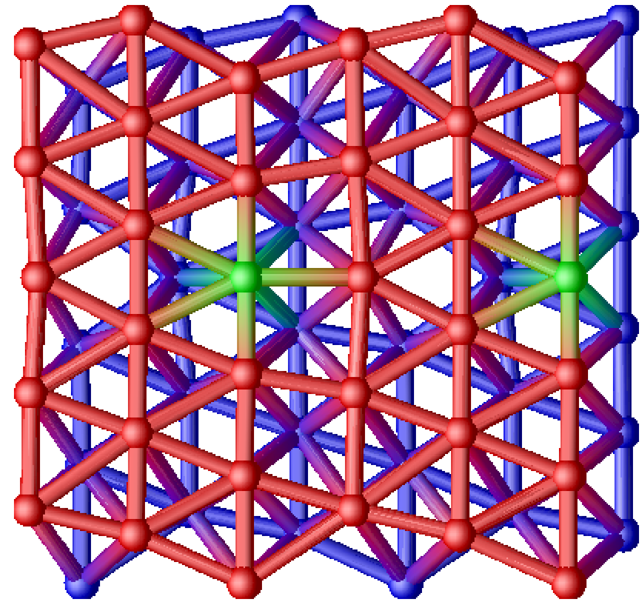
	MEAM	DFT
B1 Heat of formation	0.289eV/atom	0.290 eV/atom
L12 Heat of	1.294 eV/atom	0.359 eV/atom
L12 vol	9.693 Å^3	10.270 Å^3
L12 bulk mod	216.49 GPa	203.200 GPa
L12 c11	277.62 GPa	1556.364 GPa
L12 c12	185.927GPa	1514.88 GPa
L12 c44	91.688 GPa	63.144 GPa

V segregation at grain boundaries

sigma 3 (111) [110]

GB Formation Energy = 3.2 eV



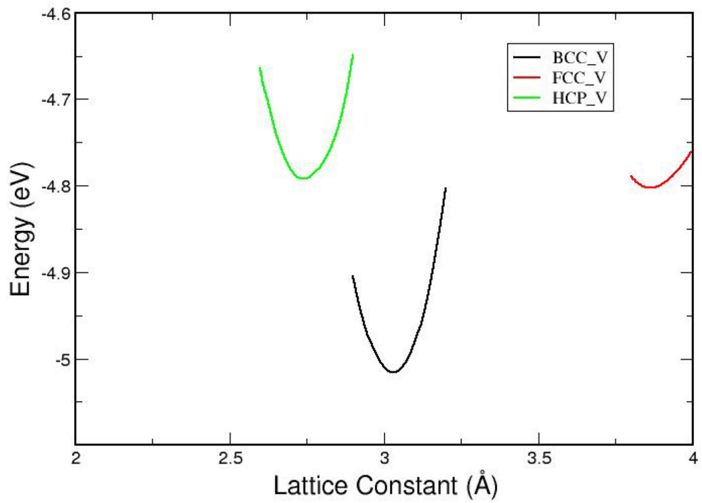


Substitutional Segregation

Interstitial Segregation

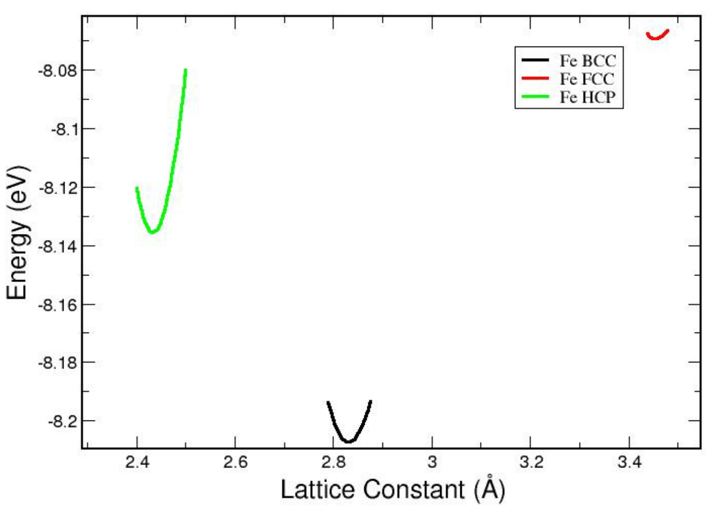
Substitutional Defect Formation Energy = -0.76 eV
Interstitial Defect Formation Energy = +1.23
Segregation Energy = -0.05

Interatomic Potential for Fe-V System



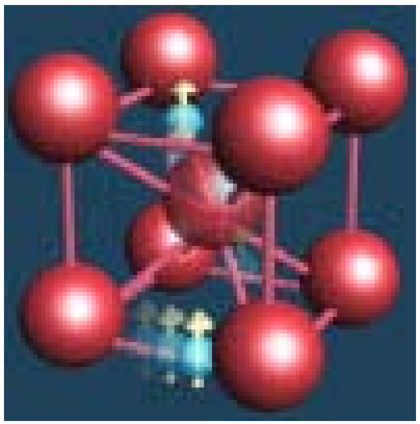
V	DFT	Expt. [a,b]	EAM
a	2.97	3.03	3.03
Ec	-8.92	-5.30	-5.01
B	96	165	162

[a] S. Han et. al. J. Appl. Phys. **93**, 3328 (2003)
[b] C. Kittel, 7th Edition

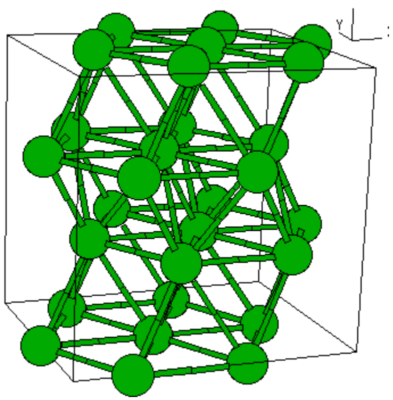


Mixed	DFT (eV)	EAM (eV)
Mono V_{Fe}	2.13	1.73
Subst.	-0.73	-0.52
Int. Oct	14.34	4.08
Int. Tet.	14.00	3.67

Ferrite Phase



bcc Fe



hcp Fe

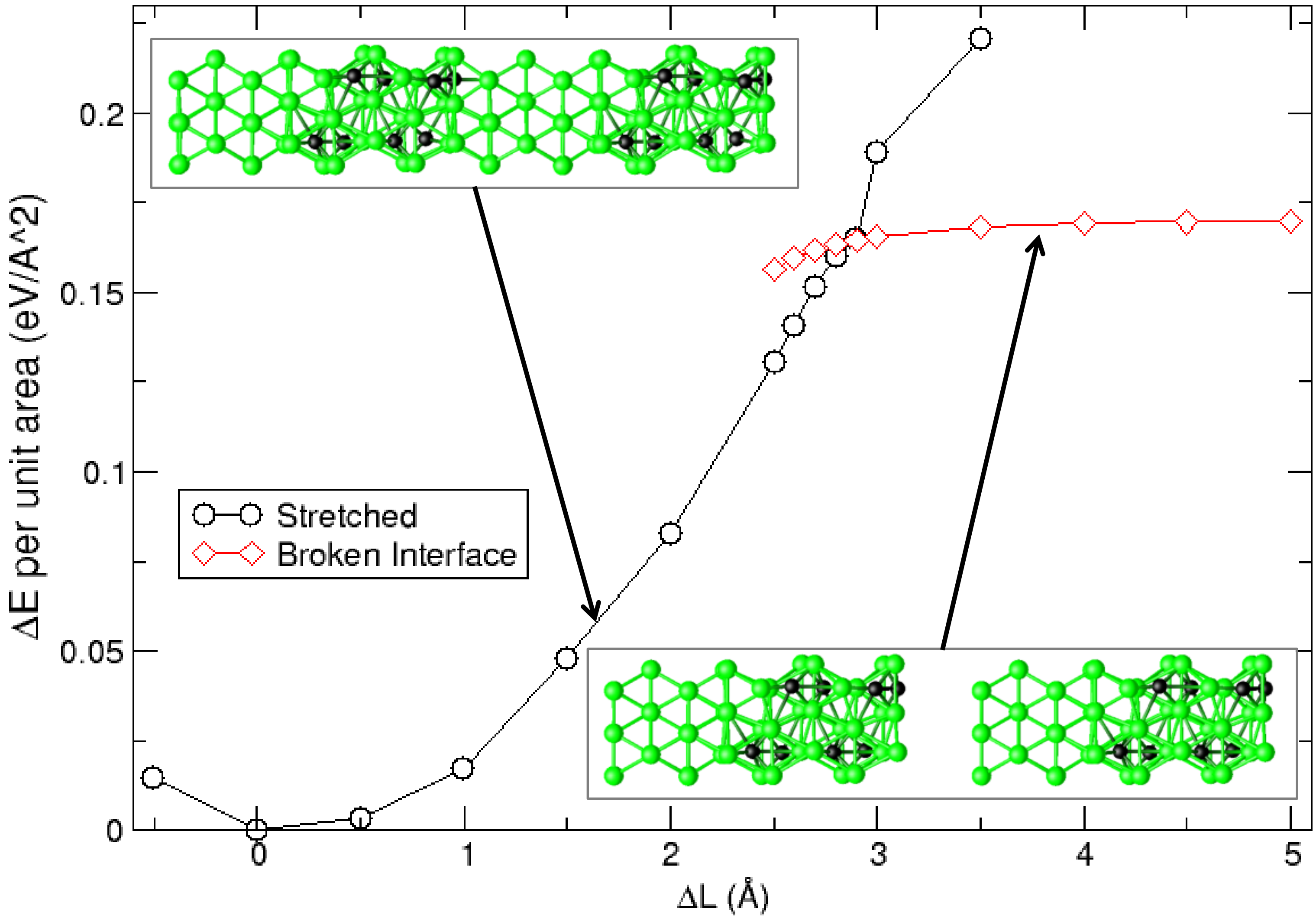
Relative energies of Fe crystals (meV)

	PAW[a]		US-PP[b]	
	LDA[c]	GGA[d]	LDA[c]	GGA[d]
bcc Fe NM	431	387	430	383
bcc Fe FM	151	**-66**	87	-238
fcc Fe NM	87	79	86	76
hcp Fe NM	0	0	0	0

[a]Projector augmented wave (PAW) method
[b]Ultrasoft pseudopotential (US-PP) method
[c]Local density approximation (LDA)
[d]Generalized gradient approximation (GGA)
NM = nonmagnetic, FM = ferromagnetic

Bulk modulus = 194.2 GPa (Exp. 170 GPa)

Cementite-Ferrite Interface



Materials Design of Steel Alloys – Dual Phase Steel Research

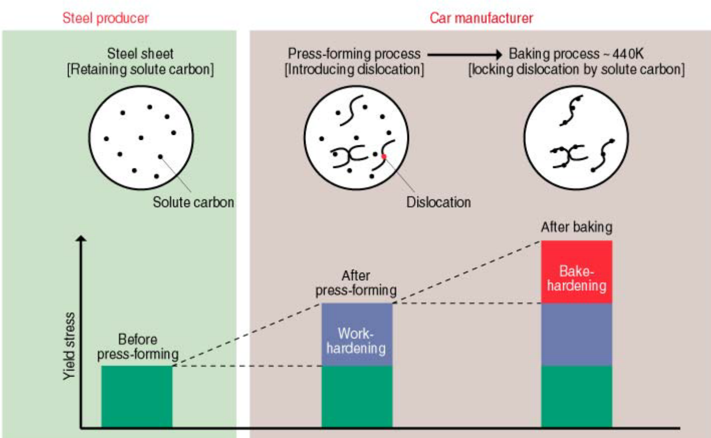
➢ DP Steels

- Low carbon high-strength low alloy (HSLA) grades
- A soft ferrite matrix (ductility/formability) + a hard martensite second phase (strength)

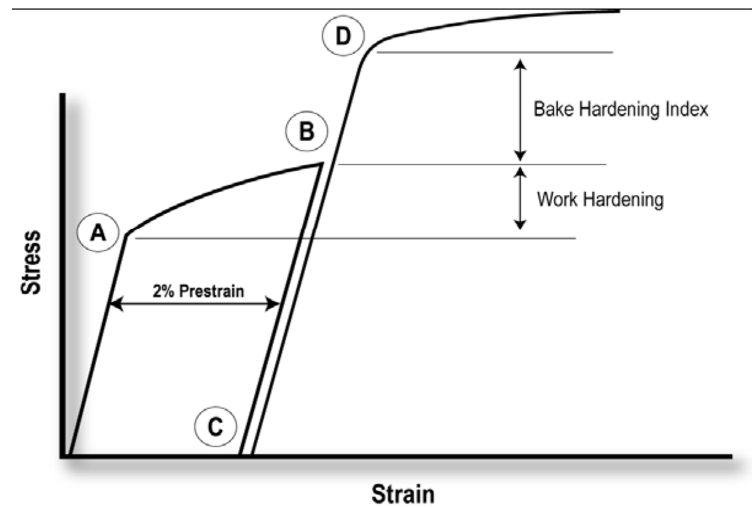
  ⇒ very attractive for automotive applications for weight reduction and formability
- Exhibit high bake-hardening (BH) effect

  : shaped into an automobile body panel (formability) & after assembly (strength)

  ⇒ not needed simultaneously !!!



[Ref.] Strength and Formability of Automotive Steel Sheets
from www.jfe-21st-cf.or.jp

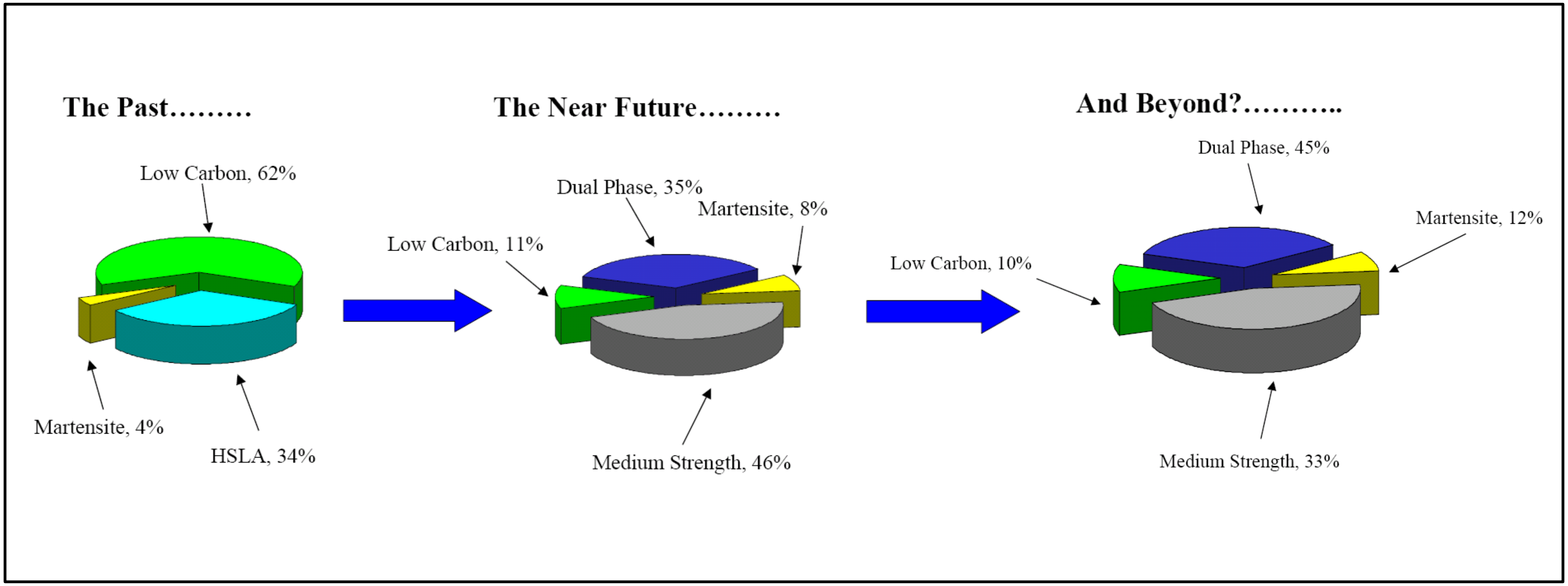


[Ref.] Advanced High Strength Steel (AHSS) Application Guidelines
from www.worldautosteel.org

dislocations introduced by press forming ⇒ work hardening (A~B) ⇒
painting & baking of automobile body ⇒ strain aging by dislocation locking (B~D)

Dual-Phase Steel Research – a pathway to develop 3rd generation AHSS

- The future of DP steels



[Ref.] C.D. Horvath, "The Future Revolution in Automotive High Strength Steel Usage"

Dual-Phase Steel - Approach

- **Material**: A DP590 steel obtained as in-kind donation

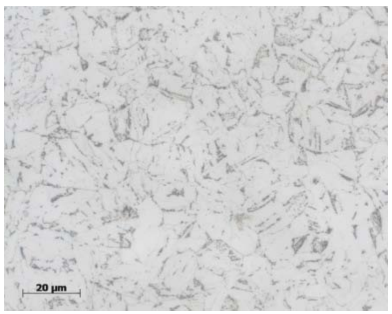
- **Experiments**
- ➢ Chemical analysis: spectrometer
- ➢ Microstructure observation: optical microscope, SEM & TEM
- ➢ Micromechanical properties: nano & micro indentation tests
- ➢ Heat treatment
  - bake-hardening: tensile specimens ⇒ pre-straining of 0 (as-received), 1, 2, & 5%
    ⇒ heat treatment (170°C, 20 min, air cooling) ⇒ tensile tests
    ⇒ SEM fractography
- - microstructure design: martensite volume fraction, ferrite grain size, micro alloying, etc.
- ➢ Quasi-static & High-rate mechanical tests: Instron & Hopkinson bar test set-ups

Dual-Phase Steel Research – Initial State

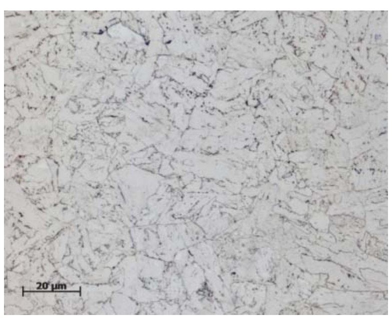
- **Chemical composition (wt%)**

C	Si	Mn	P	S	Cr	Mo	Al
0.123	0.103	1.870	0.0130	0.0046	0.008	0.061	0.049

- **Microstructure**

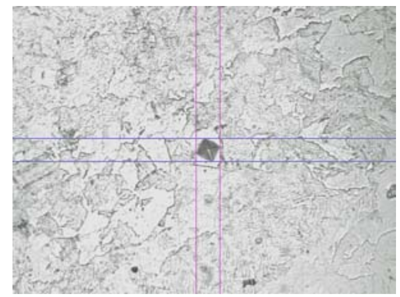


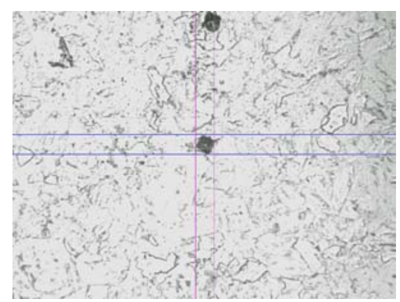
Top surface (nital, 100x)



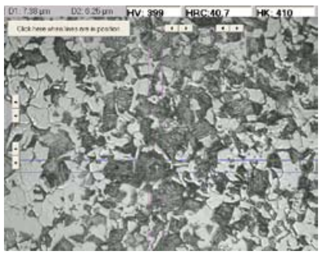
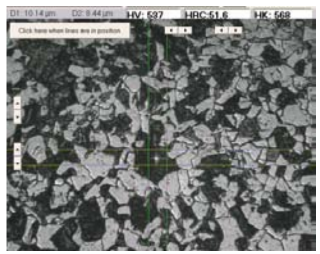
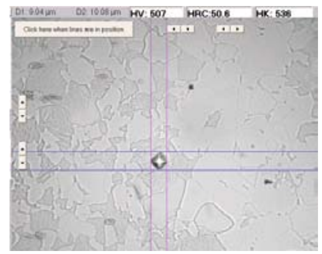
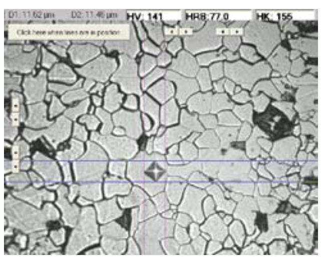
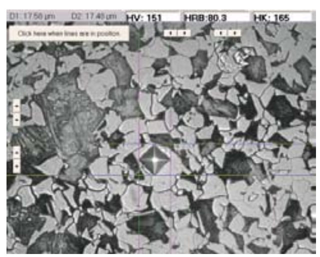
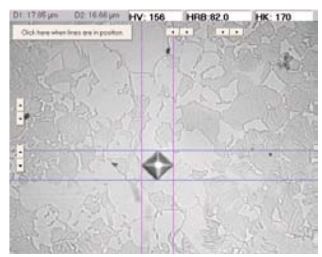
Side surface (nital, 100x)

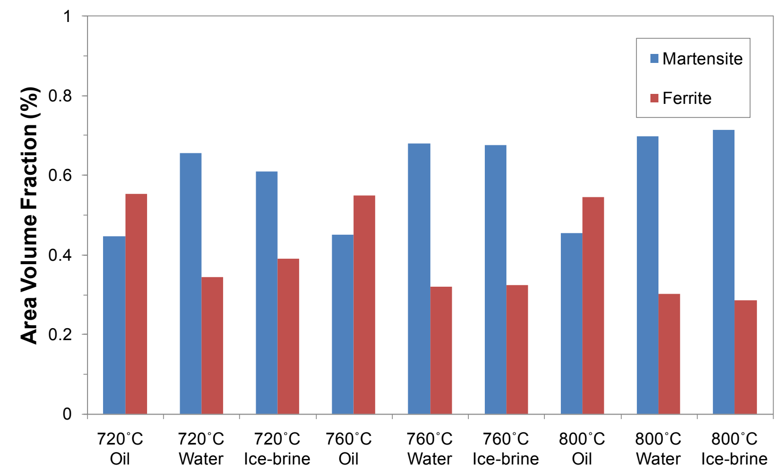
- **Hardness Comparison**

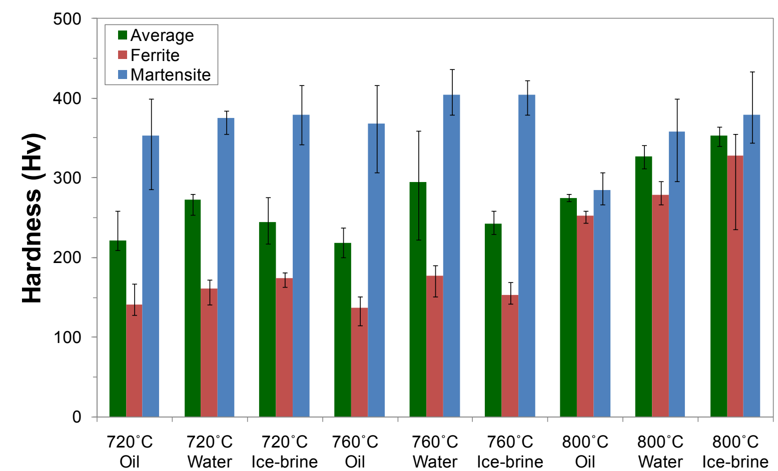

Ferrite-region
Hv = 193 (10gf, nital, 50x)


Martensite-region
Hv = 295 (10gf, nital, 50x)

Microstructure and Hardness after Heat Treatment

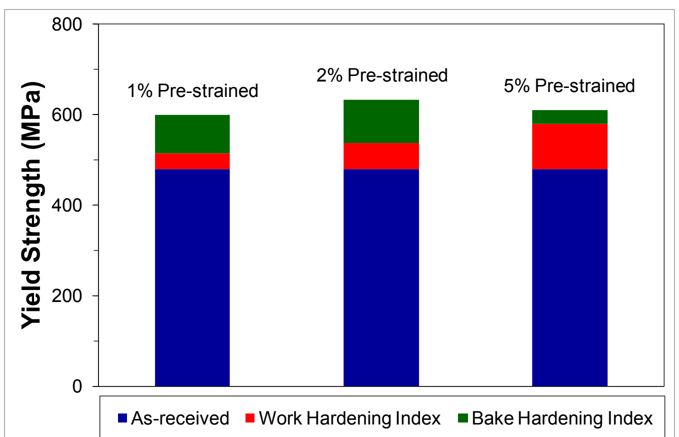
	925°C Austenizing ⇒ 760°C Annealing ⇒ Quenching		
Martensite			
Ferrite			
	Oil	Water	Ice-brine





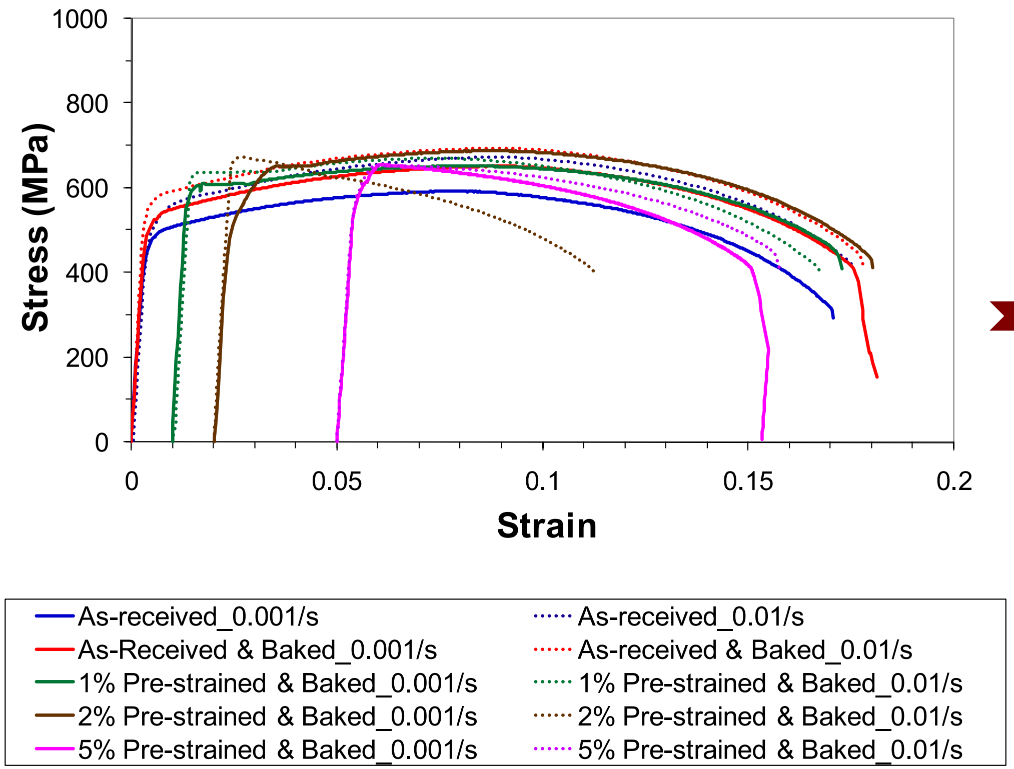
Bake hardening effect

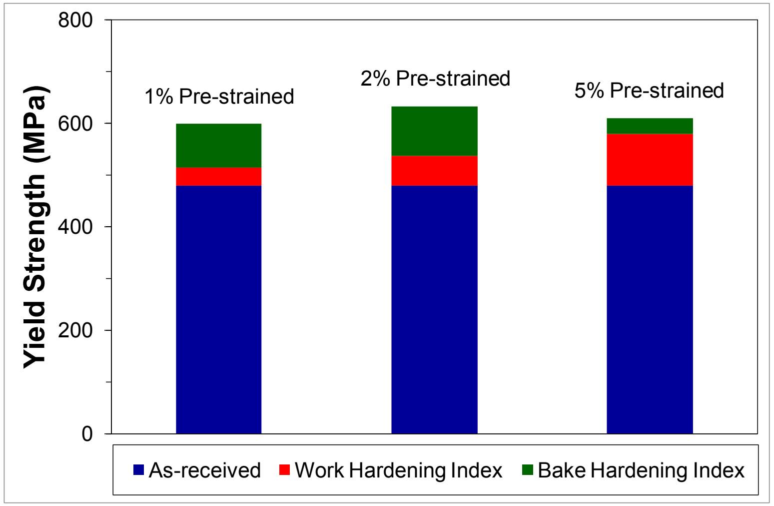
Pre-straining of 0 (as-received), 1, 2, & 5% → heat treatment (170°C, 20 min, air cooling) → tensile tests



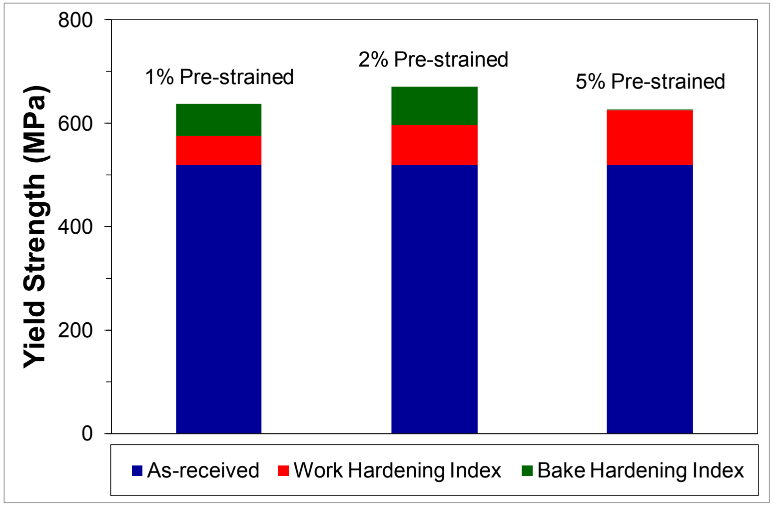
Dual-Phase Steel – Bake Hardening Effect

- **Bake Hardening Effects**





(a) strain rate = 0.001 s^{-1}



(b) strain rate = 0.01 s^{-1}

Accomplishments

1) Performed the full spin-polarized density functional theory (DFT) calculations on Fe ferrite phase to correctly account for the ferromagnetism in Fe atoms.
2) Developed a new multi-objective optimization methodology as a robust procedure to construct reliable and transferable interatomic potentials for steel alloy systems.
3) Applied the multi-objective optimization procedure to construct reliable interatomic potentials for Fe, C, and Fe-C using the force-matching-embedded-atom-method (FMEAM).
4) Obtained FMEAM interatomic potentials for Fe-V alloys.
5) Established a basic framework for the accelerated development of reliable and efficient interatomic potentials for other combination of alloy systems.
6) Performed DFT calculations of cementite Fe-C alloy phase and optimized the structure.
7) Performed DFT calculations of the diffusion of V in ferrite phase.
8) Performed DFT calculations of the diffusion of V in cementite phase.
9) Conducted fundamental materials/mechanical properties characterization and microstructure characterization on advanced high strength steel (AHSS) alloy samples obtained from POSCO, performed thermomechanical treatment and investigated the effect of bake-hardening.
10) Established a close collaborative relationship with industrial partners including POSCO, SAC, Inc., and M & S Inc.
11) Seong-Gon Kim was invited to give a keynote speech at 45^{th} Steel Technology Symposium, POSCO, Kwangyang, KOREA, July 17, 2008.
12) Many publications/presentations.

Conclusions

- The density functional theory (DFT) calculations were performed on Fe-C alloy systems using the full spin-polarized local density approximations to correctly account for the ferromagnetism in Fe atoms.
- We developed a new multi-objective optimization methodology as a robust procedure to construct reliable and transferable interatomic potentials for steel alloy systems.
- This multi-objective optimization procedure was applied to construct transferrable interatomic potentials for Fe, C, and Fe-C using the force-matching-embedded-atom-method.
- Full spin-polarized DFT calculations have been performed on ferrite and cementite phases and their interfaces.
- The effect of micro-alloying element (vanadium) – formation energy, diffusion barrier, etc. – has been investigated using DFT calculations.
- Characterized materials/mechanical properties of advanced high-strength steel alloys using dual-phase (DP) steels, performed thermomechanical treatment and investigated the effect of bake-hardening.
- This investigation should facilitate the design of new generation of advanced high-strength steels by providing fundamental understanding of several critical issues that include the selection of key combination of micro-alloying elements, interaction of precipitate and matrix phases, and ultimately composition-structure-property relationship.

Steel - Annual Deliverables

2009

- Development and validation of MEAM potentials to model lightweight alloys: Mg, Al, Mg-Al.
- Atomistic simulations of Mg-Al-Zn alloys: phi and tau phases.
- Atomistic simulations of ferrite and cementite.
- Heat treatment and mechanical tests on Dual Phase (DP) steels.
- Characterization of the nanostructure of Mg_7Zn_3Al prototype alloy by 3D atom-probe microanalysis in a Local-Electrode Atom Probe (LEAP).

2010

- Development and validation of MEAM potentials to model lightweight alloys: Fe-C.
- Atomistic simulations of micro-alloying effect: V diffusion, V segregation at grain boundaries
- The effect of altered microstructure on the strength-ductility combination of DP steels.

2011

- Development and validation of MEAM potentials to model lightweight alloys: Fe-V.
- Atomistic simulations of micro-alloying effect: V near dislocations
- The effect of altered microstructure on the strength-ductility combination of DP steels.

Timeline

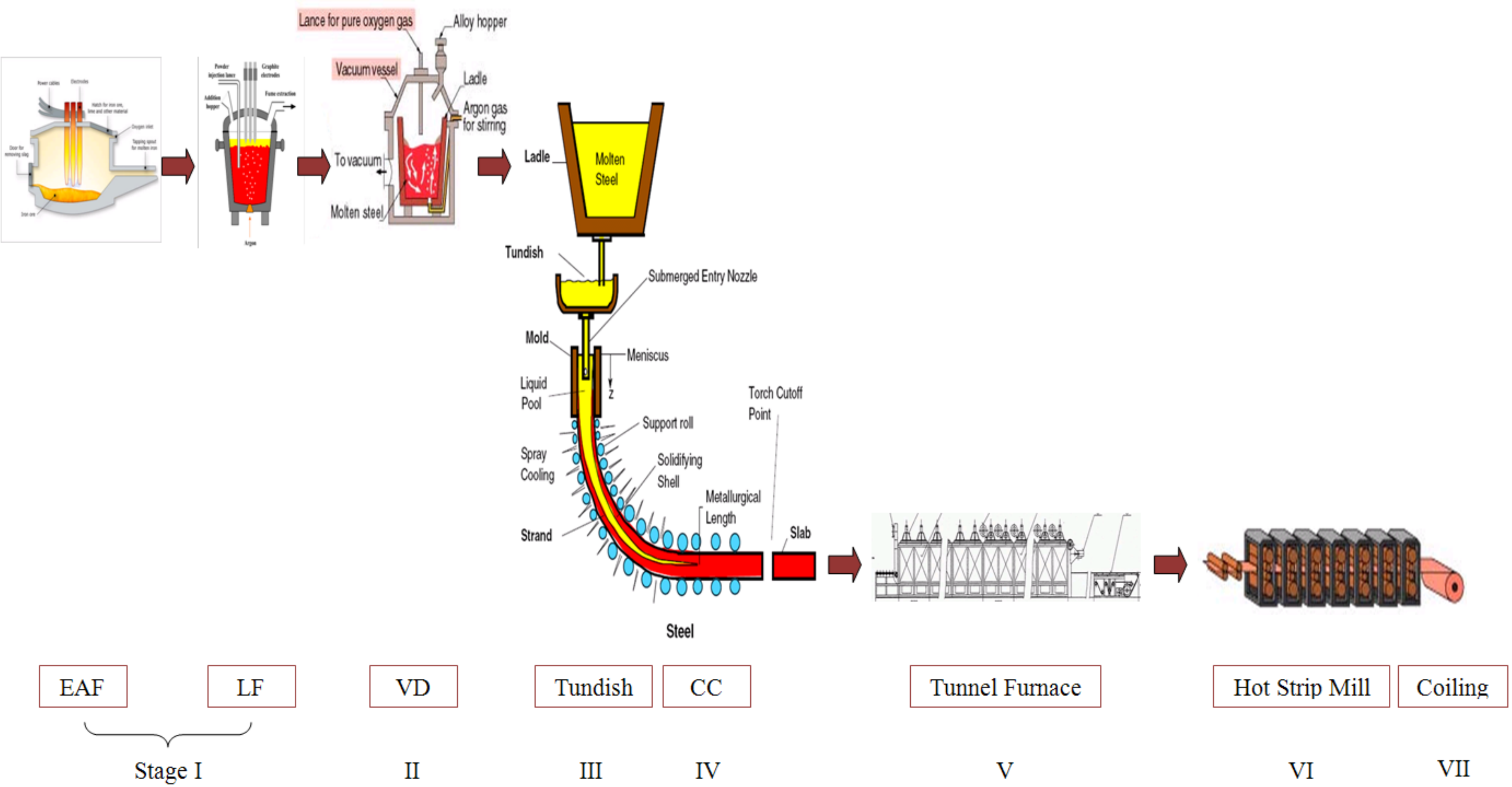
Scheduled | On Schedule | Delayed | Completed

Year	2009 (Year 1)				2010 (Year 2)				2011 (Year 3)			
Quarter	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 6. Materials Design of Lightweight Alloys												
Subtask 6.1 -- Construct and validate reliable inter-atomic potentials to model various phases of high-strength steel alloys.												
Subtask 6.2 -- Perform electronic and atomistic simulations to obtain the electronic, structural and mechanical properties of the main phases of steel alloys.												
Subtask 6.3 -- Investigate the effect of novel additives on strength and ductility of steel alloys;												
Subtask 6.4 – Investigate the effect of altered microstructure on the strength-ductility combination of steel alloys;												
Subtask 6.5 Perform experiment to test new materials and validate the results.												

Steel Manufacturing Process

(Cradle to Grace Concept)

Identify different stages of steel manufacturing plant processes. Among various commercially available mass-product steel manufacturing processes, one of the typical examples of melting, ladle refinement, micro-alloying, continuous casting, and hot rolling for thin slab direct rolling process is schematically illustrated below.



Manufacturing Cells

(Stage I & II) (Stage III &IV) (Stage V) (Stage VI)

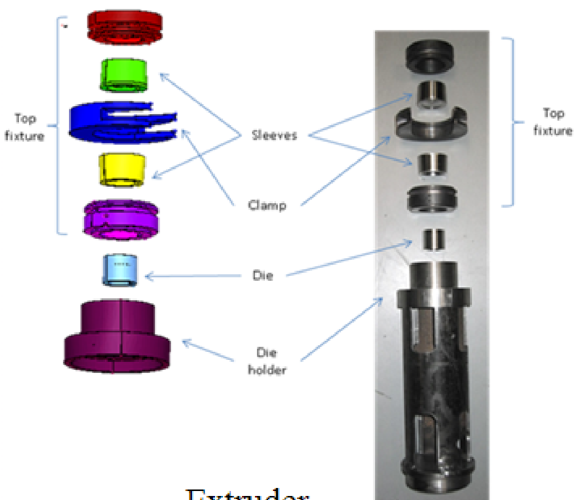
Induction Melting Furnace & Ladle

Ladle & Ingot Casting

High Temperature Re-Heat Furnace

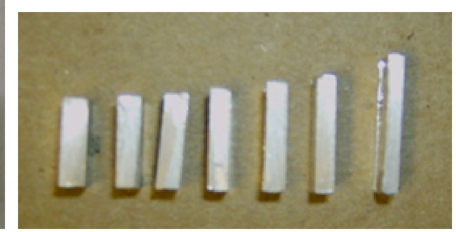
Rolling Mill

Materials/Mechanical Properties Characterization



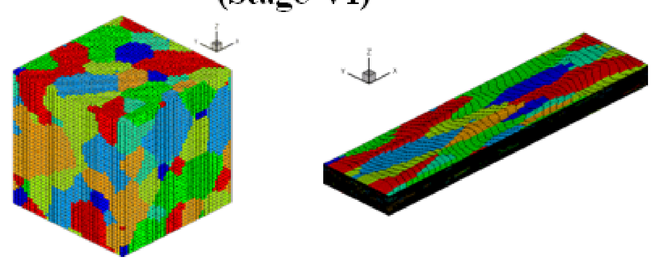
Extruder

Extruder

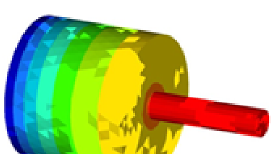


Extruded Specimens

(Stage VI)



Structure/Texture Research



FEA Simulation Research