The Foundation of Nanoscience: Multiple Length/Time Scale Modeling of Multi-physics for Nano/Micro Material System

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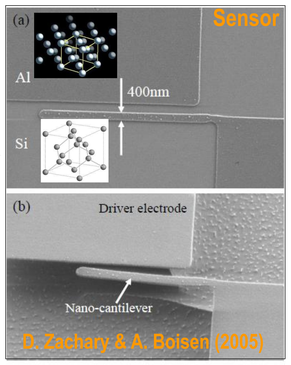
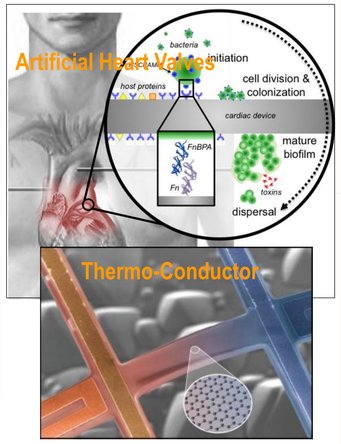
Motivation

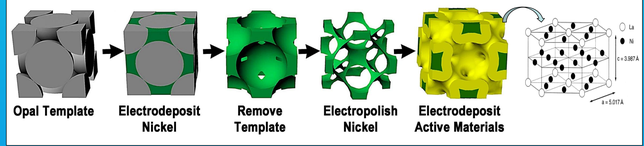
❖ Nanomaterials manifest extremely fascinating and beneficial properties, which can be exploited for a variety of applications.

❖ From design, synthesis to application of nanomaterials, **theoretical modeling of multi-physics** is at the core of the broad field of Nanoscience.





Battery



Theoretical Framework

Governing Equation: (Non-equilibrium Molecular Dynamics)

$$m^i\ddot{\mathbf{r}}^i = \mathbf{f}^i + \boldsymbol{\varphi}^i \qquad \mathbf{f}^i = -\frac{\partial V}{\partial \mathbf{r}^i}$$

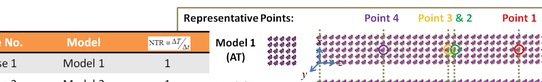
Temperature Effect (Upgraded Nosé-Hoover Thermostat) :

$$m^i\ddot{\mathbf{r}}^i = \mathbf{f}^i + \boldsymbol{\varphi}^i - \chi_{IG}(t)m^i\tilde{\mathbf{v}}^i,\ i \in S_{IG}$$

Theorem I: The total linear and angular momenta caused by the thermal velocities are vanishing;

Theorem II: The Hamiltonian remains to be constant during the entire thermomechanical process.

$$\tilde{\mathbf{v}}^i \equiv \mathbf{v}^i - \bar{\mathbf{v}} - \boldsymbol{\eta}^i \qquad \eta^i = \boldsymbol{\omega}\times(\mathbf{r}^i - \mathbf{R}_c) \qquad T_{IG} = \frac{1}{\kappa_B N_{IG}^{df}}\sum_{i\in S_{IG}} m^i(\tilde{\mathbf{v}}^i\cdot\tilde{\mathbf{v}}^i)$$



Electromagnetic Effect :

$$m^i\ddot{\mathbf{r}}^i = \mathbf{f}^i - \chi_{IG}(t)m^i\tilde{\mathbf{v}}^i + q^i\{\mathbf{E}^e(\mathbf{r}^i,t) + c^{-1}\dot{\mathbf{r}}^i\times\mathbf{B}^e(\mathbf{r}^i,t)\}$$

Classical Maxwell's Equations

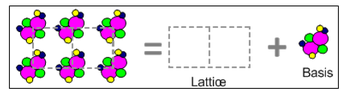
$$\nabla\cdot\mathbf{D} = 4\pi\rho$$
$$\nabla\times\mathbf{H} = \frac{1}{c}\{4\pi\mathbf{J} + \frac{\partial\mathbf{D}}{\partial t}\}$$
$$\nabla\cdot\mathbf{B} = 0$$
$$\nabla\times\mathbf{E} + \frac{1}{c}\frac{\partial\mathbf{B}}{\partial t} = 0$$

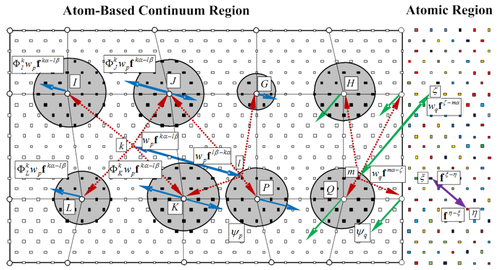
Maxwell's Equations at Atomic Scale

$$\nabla\cdot\mathbf{e} = 4\pi\sum_i q^i\delta(|\mathbf{r}-\mathbf{r}^i|$$
$$-c^{-1}\partial_o\mathbf{e} + \nabla\cdot\mathbf{b} = c^{-1}4\pi\sum_i q^i\dot{\mathbf{r}}^i\delta(|\mathbf{r}-\mathbf{r}^i|)$$
$$\nabla\cdot\mathbf{b} = 0$$
$$c^{-1}\partial_o\mathbf{b} + \nabla\times\mathbf{e} = 0$$

Non-relativistic Assumption

Lattice Dynamics: (Crystalline Materials)





Kinematic Constrain (Finite Element Approximation)

$$\mathbf{u}^{\alpha k} = \Phi_I^k\mathbf{U}_I^\alpha$$

$$\mathbf{f}^{\alpha k}\left(\delta\mathbf{u}^{\alpha k}\right) = \mathbf{f}^{\alpha k}\left(\Phi_I^k\delta\mathbf{U}_I^\alpha\right) = \left(\mathbf{f}^{\alpha k}\Phi_I^k\right)\delta\mathbf{U}_I^\alpha = \mathbf{F}_I^\alpha\delta\mathbf{U}_I^\alpha$$

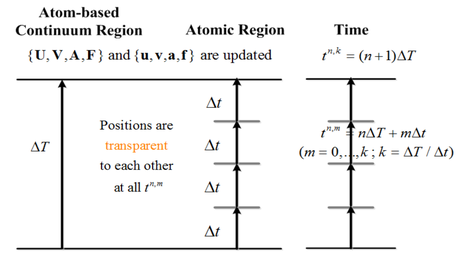
$$M_I^\alpha\ddot{\mathbf{U}}_I^\alpha = \mathbf{F}_I^\alpha(\mathbf{U},t) \qquad \mathbf{F}_I^\alpha = \mathbf{f}^{\alpha k}\Phi_I^k$$

Governing Equation: (Coarse-Grained Molecular Dynamics)

Multiple Time Scale Algorithm

Taylor Series Expansion:

$$\mathbf{U}^{n,m} = \mathbf{U}(t = n\Delta T + m\Delta t) = \mathbf{U}^0(t = n\Delta T) + m\Delta t\dot{\mathbf{U}}^0 + \frac{1}{2!}(m\Delta t)^2\ddot{\mathbf{U}}^0 + \cdots$$



Step 0: **Initial conditions**

Step 1: **Time update for the atom-based continuum region** $t = t^{n,0} = n\Delta T$

Step 2: **Time update for the atomic region** $t = t^{n,m} = n\Delta T + m\Delta t$

Step 3: **Update the displacement vectors for both regions**

$$\mathbf{U}^{n,m} = \mathbf{U}^{n,0} + m\Delta t\mathbf{V}^{n,0} + \frac{1}{2}(m\Delta t)^2\mathbf{A}^{n,0}\ ;\ \mathbf{u}^{n,m+1} = \mathbf{u}^{n,m} + \Delta t\mathbf{v}^{n,m} + \frac{1}{2}(\Delta t)^2\mathbf{a}^{n,m}$$

Step 4: **Compute the interatomic force and acceleration for atomic region**

$$\mathbf{a}^{n,m+1} = \mathbf{a}(\mathbf{u}^{n,m+1}, \mathbf{U}^{n,m+1}, t^{n,m+1})$$

Step 5: **Update the velocity vector for atomic region** $\mathbf{v}^{n,m+1} = \mathbf{v}^{n,m} + \frac{1}{2}\Delta t(\mathbf{a}^{n,m} + \mathbf{a}^{n,m+1})$

Step 6: **Update counter** $m \leftarrow m+1$

Step 7: **Go to step 2 unless** $t = (n+1)\Delta T$

Step 8: **Compute the interatomic force and acceleration vectors for atom-based continuum region**

$$\mathbf{A}^{n+1,0} = \mathbf{A}(\mathbf{U}^{n+1,0}, \mathbf{u}^{n+1,0}, t^{n+1,0})$$

Step 9: **Update the velocity vector for the atom-based continuum region**

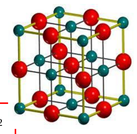
$$\mathbf{V}^{n+1,0} = \mathbf{V}^{n,0} + \frac{1}{2}\Delta T(\mathbf{A}^{n,0} + \mathbf{A}^{n+1,0})$$

Step 10: **Update counter** $n \leftarrow n+1$

Step 11: **Output the results; if simulation not complete, go to Step 1**

Implementation Flowchart

Database for MgO



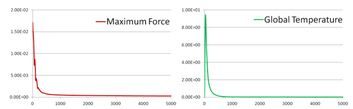
Coulomb-Buckingham Potential:

$$V^{ij} = \frac{q^iq^j}{r^{ij}} + A^{ij}e^{\frac{-r^{ij}}{B^{ij}}} - C^{ij}\left(r^{ij}\right)^{-6} + D^{ij}\left(r^{ij}\right)^{-12}$$

	A	B	C	D	Short Range	Long Range
Mg-O	47.2	0.566	0	0	12*A (A=1.889726 Bohr)	4*12*A
O-O	350.88	0.414	54.09	2463.2		
Mg-Mg	0	0	0	0		

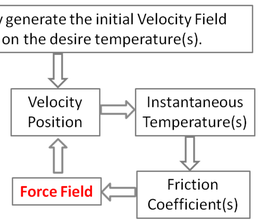
Numerical Simulation Procedure

Stage I: Relaxation (Minimize the total energy for the whole system)



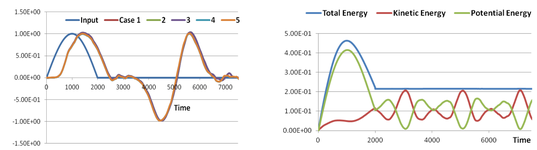
Stage II: Isothermal Control T_{est}

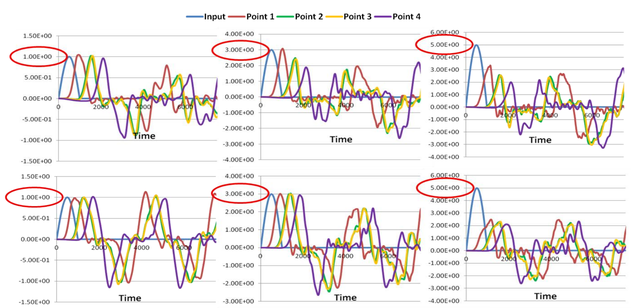
Stage III: Solving the Governing Equations



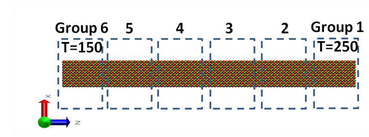
Sample Problem #1 Mechanical Wave Propagation

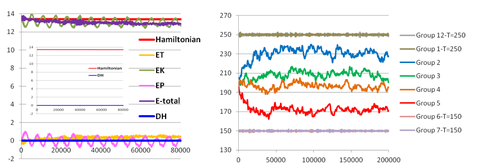
Case No.	Model	NTR = Δt/Δ_0
Case 1	Model 1	1
Case 2	Model 2	1
Case 3	Model 2	4
Case 4	Model 3	1
Case 5	Model 3	4

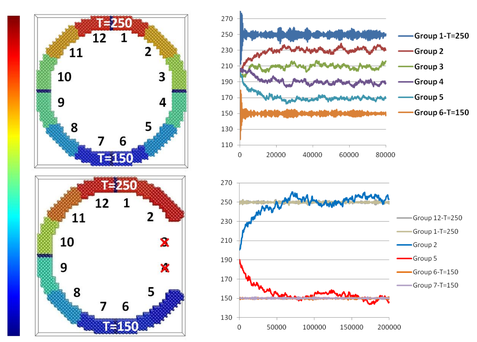




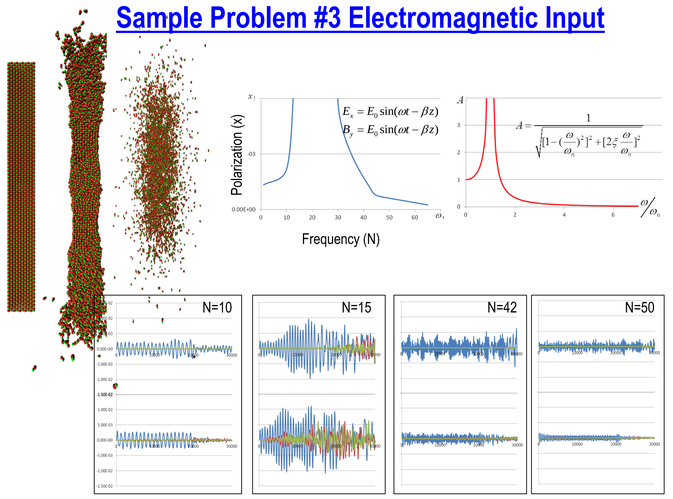
Sample Problem #2 Heat Conduction







Sample Problem #3 Electromagnetic Input



Acknowledgements

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