**Advanced Materials Thermodynamics**

Thermodynamics for Materials Scientists.

There is no such state as enlightened retirement, where we can live on the bounty of past attainments.

Wisdom is alive only as long as it is lived, understanding is liberating only as long as it is applied.

C. Feldman and J. Kornfield

Prof. Greg Beaucage, gbeaucage@gmail.com

Textbook: Chemical Thermodynamics of Materials

Macroscopic and Microscopic Aspects

Svein Stølen and Tor Grande (with Neil L. Allan)

Class Meets Tuesday and Thursday 12:30 to 1:50 Passcode "1"

Location: ZOOM (click link above)

**Thermodynamic Foundations ppt**

Videos: T220823 passcode 4R59.mwd, R220825 passcode 3?!3SiUD

8/27/2020, 9/03/2020 Thursday

Homogeneous vs Heterogeneous Ceramics

Heterogeneous Cermet for Constant Resistivity with T

Homogeneous Mg Silicate fibers from electrospinning

Gluten Phase Separation

Non-Ergodic Material

Simulation: Helmholtz and CV concrete (https://en.wikipedia.org/wiki/Quasi-harmonic\_approximation)

Ceria Oxide Heat Capacity and Gibbs FE Calcuation from Measurements for surface components

Size-dependent Melting point for energy storage materials

Hess' Law for Surface Absorption

Reversible Laminar Flow, Before and After

Supercooled Water Tricks

Gibbs-Duhem and Chemical Potential for Corrosion of Nanoparticles

First Order Transition Curie for Cancer Treatment

Modulated DSC

**Single Component Systems**

Videos: T830 n%FJ8NFY; R901 ?J&D07sB

T906 iA2h=Hu@ ; T908 3fF29vk!

9/08/2020 , 9/10/2020, 9/15/2020 , 9/17/2020

Ice Phase Diagram at High Pressure

Clausius Clapyeron for Absorption Enthalpy of Hydrogen on Carbon

Glass Transition as a Function of Pressure

Tg for single molecule particles and entanglements; Flory Fox Paper

Supercritical Fluid Video, Supercritical Production of Aerogel Video

Gelation as a second order phase transition

Ising Model, Ising and Monte Carlo Wikipedia, Classes of Magnetic Materials

Ising Model for Stacked Graphene

Robert A. Alberty, J.Chem.Thermodynamics2002,34,1787–1823

ThermoCalc for Mac/PC; Open CALPHAD for PC

Landau for alpha beta transition in quartz

Peng-Robinson Equation of State.xls (PREOS)

PV diagram for Solid/Liquid/Vapor/Supercritical Fluid

Excluded Volume for Cylinders and Nanotubes (1984 718 citations)

Ex. Vol. of CNTs 2007

Moire superconductive graphene Landau

**Solutions**

Videos: T220913 TC=$+95=; R220915 w1.=gz\*7

9/22/2020 , 9/24/2020

Activity Coefficient Bismuth/Lead Heat Transfer Fluid

Predicting Activity Coefficients for Electrolytes

Asphaltene Activity Coefficient

Activity Coefficients for Polyhydroxybutyrate Using Inverse Gas Chromatography

Hildebrand Solubility Parameter CNT/Polymer

Del from Chi Parameter for Drugs in Polymers

Tg and activity coefficents; Gordon Taylor Model; Review of Tg solution models

**Phase Diagrams**

Videos: R220920 Y6=BmKpK ; T220922 0BD%mQ98

9/29/2020 , 10/1/2020

Globular to Lamellar Transition in Eutectic Alloys

Construction of a phase diagram SiO2 V2O5

Calculation of a Phase Diagram KCl NaCl

Bi-Zn Solder

Ternary free energy expression

La Ni Fe phase diagrams Eutectics

PVME/PS Phase Diagrams; PVME/PS Phase Diagrams 2; PVME/PS Phase Diagrams 3

Nanoparticles and PVME/PS Phase Diagrams

Additive Manufacturing of Nickel Alloys

Growth of Intermetallics

Inconel 718 Phase Structures for Ni alloys

Defects in Additive Manufacturing of Ni Based Alloys

CALPHAD calculation for nano AgCu

High Pressure phase diagram for Ti64

Phase Diagrams Globular to Lamellar Transition in Eutectic; Ab initio calculation of EUtectic using DFT 2022; Simple Density Functional Theory; Neural NEtwork for potentials; Simple explaination of functionals; Machine Learning; ; Ferrielectric ferroelectric transition; Austinite crystal orientation 111 110; Eutectic Nature; Deep eutectic for concentrated solar

Phase **Stability**

Videos: T220927 7$hT1L$E; R220929 TDuV1+E\*

10/6/2020 , 10/8/2020, 10/13/2020

Fluctuations

Spinodal Decomposition Hashimoto PVME/PS

Spinodal Beaucage A, Beaucage B

Spinodal Polymer Notes, Lab

Spinodal Pictures A, B

Strobl Chapter 4 Polymer Physics (add "f" at end)

Simulation of Spinodal

Higgins Tacticity

Higgins Spinodal

Hashimoto Spinodal Curvature

Spinodal in Polymer Network

Spinodal for various free energy expressions

Use of Cahn Hilliard to model cell growth

Modeling Nucleation and Growth

Antifogging spinodal

Dust Proof spinodal

Spinodal 2022

Shape Depencdent Phase Separation Sharon Glotzer

Cahn Hilliard with anisotropy for membranes

2006 Spinodal Simulation for Membranes

**Surfaces**

Videos: T20221004 Gew.hs1. ; R20221006

10/15/2020, 10/20/2020, 10/22/2020

Grinding Limit for Particles

Adamson Physical Chem of Surfaces

Hiemenz Surface Chemistry 1997

Surfaces Israelachvili

Soft Interfaces de Gennes

Thermodynamics of Materials (Surfaces, Statstical, Interfaces)

Nanoparticle Course

Industrial Crystallization from Solution Mersman

Crystallization in Confinement 2021

Stability of Nanobubbles

Ion Stabilized Nanobubbles

Nanobubbles in Nuclear Fuel

Nucleation of Gold Nanoparticles

Fibers to Protect Nanoparticles

Adsorption versus Absorption (short video)

Review on BCP Templated Ceramics, Metals, and Carbons for Batteries

Block Copolymers Hamley

Strobel Polymer Physics

Meier 1969 BCP phase size

Rubeinstein Colby Polymer Physics

Surfactant Science

BET Theory

Nanotube Adsorption

Intercalated Dye Adsorption

Supercritical Adsorption

Gregg Sing Adsorption Surface Area

Keller Staudt Gas Adsorption 2005

Suplemental 1 Surface nucleation of ice by Maching Learning

Supplemental 2 for Ice

Ice Machine Learning Paper

**Enthalpy of Formation**

Videos: 10/27/2020, 10/29/2020

Perovskite Growth Video

Construct a Perovskite Solar Cell

Perovskite Video

Zeolite Paper 2000

Zeolite 1995

Intermetallic substitution for hydrogen storage

Polymer Physics Resource

Rotational Isomeric State Model 1

Rotational Isomeric State Model 2

RISM University of Twente

**Heat Capacity**

Videos: 11/03/2020 , 11/05/2020, 11/10/2020, 11/12/2020

Acoustic and Optical Modes Demonstration

Cp from IR and Raman

Cp from Group Contribution

Dependence of Entropy on Molar Volume(ref 15)

Metal Insulator Transition Review

Spinel, Perovskite, and Rutile

Another Spinel, Perovskite, Rutile page

Einstein-Debye Function and Tarasov Model

Heat Capacity of Polymers

Calculations for the Heat Capacity of Polymers

Heat Capacity for Semi-Crystalline Polymers Wunderlich

Wunderlich 1995

Stiffness and Debye Temperature for Boron Nitride and Carbon Polymorphs

Quasiharmonic Calculation of Heat Capacity for Ni and Ni3Al

(Wang-Debye Model)

Heat Capacity of Gold Nanoparticles on Carbon Nanoparticles

Heat Capacity of Nanoparticles

**Atomistic Solution Models**

Videos: 11/17/2020, 11/19/2020

Mean field and specific interactions

Quasi-Chemical Model

Spintronics

Semi-metal

Stat. Mech. of Soft Core Fluid Mixtures (introduction is good review)

Diffraction study of nanosize Gahnite ZnAl2O4 (spinel)

Perovskite Solution Model by Stolen (book author)

Stabilization of nanocrystalline binary alloys (Regular Solution Model with defects)

Alloy Effects in Nanostructures (1993)

Alloy thermodynamics in nanostructures (1994)

**Experimental Thermodynamics**

Videos: 1/2/2020

Differential Thermal Analysis Low Temperature

Modulated DSC TA Instruments.pdf

Modulated DSC Summary.pdf

Artifacts in DSC.pdf

TA DSC and PET Modulated DSC.pdf

TA Modulated DSC and PET.pdf

Microcalorimetry for Batteries 1

Microcalorimetry for Batteries 2

Microcalorimeter Instrument

Thermal Gravimetric Analysis for Tires TGA A.pdf , TGA B.pdf

TGA for BioChar Talk; Paper on Bamboo TGA

Kissinger Equation for TGA (and DSC)

**Thermodynamics and Materials Modeling**

Videos: 11/24/2020

Example LAMMPS code

Computational Methods in Physics (Extensive Webpage)

Compare LAAMPS and HOOMD

Review 2009 Dissipative Particle Dynamics

Review 2015 DPD

DPD Review 2017

Perturbation Methods

DPD Karniadakis Talk

DPD with LAMMPS Talk

DPD Groot Talk

Groot Lecture Notes

Espanol Warren Review

DPD Polymers Spenley

Polymer Dynamics Review Padding

Army ARL EPDP Lecture

LAMMPS; ESPResSo; HOOMD-blue; DPDmacs; MyDPD; coLAB

LC Assembly Movie

**Course Review**

Videos: Course Review 12/1/2020

**Course grade weekly homework**