UG Final Year Projects for

2014-15

Vikram Jayaram

Fracture toughness using a clamped beam bend geometry

Recently, a new geometry has been developed that allows for stable crack propagation under constant load, i.e., keeping the load fixed, the crack driving force actually drops as it propagates. This feature was identified during thin film testing but should, in principle, be applicable to any sample size. If so, it will allow ready toughness determination of many difficult classes of materials, in particular those that are somewhat brittle and show crack resistance curves. This project will combine fabrication of samples with mechanical testing coupled with finite element analysis to develop this technique towards routine application. Depending on interest, the project can be biased towards either modeling or experimentation.

References:
(a) Nagamani Jaya B, Vikram Jayaram and Sanjay Kumar Biswas: A new method for fracture toughness determination of graded (Pt,Ni)Al bond coats by microbeam bend tests, Phil. Mag. A Volume 92, Issue 25-27, pages 3326-3345 (2012)

(b) N. J. Balila and Vikram Jayaram: Crack stability in edge notched clamped beam specimen under bending: Modeling and experiments Int. J. Frac. (in press, I can provide a copy if anyone is interested)

Kaushik Chatterjee

Processing materials for biomedical applications

The current work in the lab encompasses a variety of material systems for biomedical applications. We work on bulk and surface processing of Ti alloys for use in orthopedic implants. We develop biodegradable polymers for drug delivery and tissue engineering. We also work on nanocomposites wherein nanoparticles are incorporated in polymer matrices for tissue engineering applications. All these projects involve two components- material processing and study of biological response to these materials. UG students interested in joining the lab can choose to work on any of these topics based on their interests after discussion with the faculty.

Suryasarathi Bose

EMI shielding materials derived from PVDF and 2-D graphene sheets

In recent wireless era, the usage of electronic equipments and communication devices has increased tremendously. As electronic industry advances, new type of pollution is increasing through electromagnetic (EM) radiation emitted from the electronic systems. This pollution is primarily responsible for inefficiency of equipments and also has an adverse effect on the human health. In order to protect the work space and equipments from electromagnetic radiation, development of new materials which can absorb or reflect the EM radiation have become indispensable. Polymers have high dielectric strength, flexibility, easy process ability and low processing temperatures. Hence, polymer based nanocomposites are best suitable for shielding applications as it can maintain a good working environment of the devices. The other important key properties for EMI shielding materials are the presence of magnetic dipoles in the system. The primary objective of this work is to design nanocomposites with very high EMI shielding effectiveness. This can be achieved through homogeneously dispersing intrinsically conducting particles like thermally reduced graphene sheets (rGO) in a polymer matrix (here Poly (vinylidene fluoride), PVDF) which can attenuate the EM radiation through reflection and absorption. In addition, nanoparticles with magnetic dipole will be introduced that can further absorb the magnetic field associated with the EM radiation. To accomplish this concept, rGO will be grafted with Fe_3O_4 nanoparticles and due to its high surface area and magnetic nature. Uniform dispersion and network formation of rGO grafted with INPs can lead to synergetic effect which can further result in higher attenuation of EM radiation. Thus flexible nanocomposites can be developed for shielding EM radiations.

References:

Huo, J., L. Wang, and H. Yu, Polymeric nanocomposites for electromagnetic wave absorption. Journal of materials science, 2009. 44(15): p. 3917-3927.

Colaneri, N.F. and L. Schacklette, EMI shielding measurements of conductive polymer blends. IEEE Transactions on Instrumentation and Measurement, 1992. 41(2): p. 291-297.

Kim, S. W.; Yoon, Y.; Lee, S.; Kim, G.; Kim, Y. B.; Chun, Y. Y.; Lee, K., Electromagnetic Shielding Properties of Soft Magnetic Powder–Polymer Composite Films for the Application to Suppress Noise in the Radio Frequency Range. Journal of magnetism and magnetic materials, 2007, 316, 472-474.

N. Ravishankar and T.A. Abinandanan

Calculation of Equilibrium Shapes of Alloy Nanoparticles

The equilibrium shape of a crystal can be calculated using the celebrated Wulff construction once the value of the surface energies of the facets can be calculated. In this project we will use both analytical methods and kinetic Monte Carlo methods to determine the equilibrium state of alloy nanoparticles in systems that show a negative heat of mixing (ordering tendency). The results are expected to be important for determining the shape, structure and composition distribution of alloy nanoparticles that are used for catalytic applications.

Chandan Srivastava

Controlled Manipulation of Electrical and Magnetic properties of Graphene-Nanoparticle Based Composites

Graphene is a two dimensional material made up of densely packed carbon atoms through sp^2 hybridization [1]. Graphene has received wide technological attention due to its exceptional optical, mechanical, thermal and electronic properties which have applications in fields such as fuel cells, solar cells, lithium ion batteries, gas sensors, super capacitors, composite materials, catalysis, drug delivery etc. [2]. This project will involve engineering of electrical and magnetic properties of graphene-nanoparticle based composites. Graphene will be synthesized using the electrochemical exfoliation technique [3]. Nanoparticles/nanorods will be synthesized using the wet chemical synthesis or electrodeposition techniques. Electrical properties will be manipulated by incorporating defects into the graphene by methods such as chemical treatment of the graphite electrode or incorporating defect into the graphite electrode used for the electrochemical exfoliation experiment. Magnetic properties will be tuned by manipulating shape, size, composition and morphology of the magnetic nanosolids. This project will provide an exposure in the areas of synthesis of nano-solids and graphene, electrochemistry, structural characterization techniques and techniques related to the characterization of magnetic and electrical properties of materials.

[1] Geim AK, Novoselov KS. The rise of graphene. Nature Materials 2007;6(3):183–91.
[2] Geim AK, Graphene: Status and Prospects. Science 2009; 324: 1530-1534.
[3] K. Parvez, Z. S. Wu, R. Li, X. Liu, R. Graf, X. Feng, and K. Müllen. Exfoliation of Graphite into Graphene in Aqueous Solutions of Inorganic Salts. Journal of American Chemical Society 2014; 136: 6083-6091.

Rajeev Ranjan

Ferroelectric based electrocaloric materials

Oxide perovskite based ferroelectrics materials are among the most extensively used and investigated electronic ceramics. These materials exhibit interesting and technologically important functional properties such as piezoelectric electro-optic, magnetoelectric, electrocaloric, etc. These properties can be tuned by suitable chemical modification and varying the processing conditions can be fabricated in the form of bulk ceramics or thin film forms, each having their own interesting peculiarities. One of the recent attractions with regard to these materials is related to their interesting electro-caloric (EC) properties (Moya et al, Nature Mater 13, 439 (2014). The phenomenon of EC analogous to magneto-caloric and mechano-caloric where switching on/off of the stimulus (pressure, magnetic/electric field) is accompanied by change in temperature of the material. Such materials are used in cooling/heating devices and have tremendous market potential. In this project it is intended to synthesize the material in lab, carry out structural, microstructural, ferroelectric, dielectric characterization and develop instrumentaton for electrocaloric measurements.

Govind Gupta
(3 projects)

1) **Development of Graphical User Interface for Heat Treatment Process**
Many good scientific works go unnoticed due to bad way of disseminating the information. Presenting the scientific findings in more simplified and attractive way is the demand of the industry and public. Therefore, numerical results can be conveyed very effectively to any one using object oriented framework. Usually Object Oriented Programming (OOP), such as Visual Basic (VB), Visual C^{++} and JAVA, is used to create graphical user interface for any process. Mostly scientific computer codes, written in Fortran, Pascal or C, are developed in non-interactive mode i.e. all the events in the program occur in a sequential manner. In interactive programming, as it is used in object oriented programming, the user initiates all the events and decides in what order they should occur. Therefore, additional efforts for programming are needed. In the present work, one would be developing a graphical user interface for the gas carburizing process using Visual Basic/ Visual C^{++}/JAV. Specific tasks such as programming to view graphical information, to control window operations and to process user feedback would be incorporated using graphics libraries and developing the appropriate programs.

2) **Characterization of indigenously produced silicon carbide powder**
As the name suggests, one has to study the morphology of the silicon carbide powder which is produced indigenously in our laboratory. One has to use SEM, XRD, TEM, EDAX, etc to characterize the powder. To determine the various elements in the powder, one has to use chemical analysis method.

3) **Solid flow modeling using DEM**
Using discrete element method (DEM), one has to model solid flow either in a Blast furnace or pipe or in silo. Using this approach one can study these flow more fundamentally and accurately. This approach can be combined with CFD (computational fluid dynamics) such as gas flow to study the two-phase flow.

Praveen Kumar

Effect of interlayer on electric field induced failure in thin metallic structures

Electric current of high densities forces the atoms in a solid metal to migrate along the direction of electron flow; this phenomenon is called electromigration. It is driven by the momentum transfer from colliding electrons to ion cores of an atom and its kinetic is controlled by diffusion. It is one of the major challenges faced by the microelectronic industry. In very thin films, the effect of interlayer between the metallic film (such as Cu) and the substrate (such as Si) may influence the diffusion as well as the electron flow; we would like to study how the interlayer affects the electromigration and the reliability of a microelectronic device. The work is mainly experimental and it will involve thin film deposition and relevant testing techniques.

Dipankar Banerjee and Praveen Kumar

FEM Analysis of this foil relaxations in TEM samples of Ni Base superalloys

Ni base superalloys used in Turbine blades of jet engines consist of 2-phase gamma/gamma prime microstructures. A important parameter determining the properties of these superalloys is the misfit between between the gamma and gamma prime phases. The determination of misfit often relies on determining accurate lattice parameters in thin foils by convergent beam electron diffraction (CBBED) or by digital analysis of lattice images. However the determination of misfits by these techniques is subject to relaxation of local stresses due to relaxation in the thin foils. The objective of this project is to determine the extent of relaxation by FEM techniques that will model the two phase structures and evaluate the effect of foil thickness on the degree of relaxation. The project will involve understanding the FEM techniques in relation to this project and and applying the techniques appropriately to obtain the desired results. If time permits. We may attempt to validate the results by CBED on thin foils of Ni base superalloys.

Abhik N. Chaudhury

Influence of solutal convection on the scaling behavior of lamellar spacing under directional solidification conditions

Eutectic solidification offers a nice example for understanding pattern formation in multi-phase solidification. An important phenomena that is essential to the investigation of formation of micro-structures, is the role of convection. In this present work, there are two main aims. Firstly, we incorporate buoyancy driven flow in an already existing phase-field code, in order to model phase transformation coupled with flow in two dimensions. Only solutal driven convection will be considered in this example. Secondly, the implementation will be utilized to perform a parametric study wherein, the under-cooling at the interface will be derived as a function of spacing for different velocities and temperature gradients. The results will be compared with simulations performed without convection and the classical Jackson-Hunt analysis. Finally, effect of solutal convection on the spacing selection in large lamellar arrays, upon initiation of long-wavelength perturbations of the lamellar front, will be studied. The work will be useful in the eventual investigation of pattern-formation in bulk 3D samples.

References:

1) Applied Mathematical Modelling 28 (2004) 109–125

2) Journal of Crystal Growth 222 (2001) 365–379

3) Acta Materialia 57 (2009) 2640–2645

4) PHYSICAL REVIEW E 61(2000) R49-52

S. Karthikeyan

Creep and microstructural studies in vanadium alloys for future fusion reactors

It is common knowledge that fossil fuels will not be able to meet future energy demands and that the greatest challenge today is to identify viable renewable and environmentally friendly alternatives. An exciting area of energy research is aimed at realizing the potential of nuclear fusion (yes, fusion! As in ${}_1^2H + {}_1^3H \rightarrow {}_2^4He + {}_0^1n$ + whole lot of energy!). Fusion promises a virtually inexhaustible source of clean energy. More details on the viability, advantages and challenges facing fusion reactors can be found at http://www.iter.org/. In brief, the primary challenge to fusion reactors is that presently we have neither the technology nor the materials. Materials for future fusion reactors will be required to withstand extremely high temperatures and radiation doses. These conditions can lead to severe radiation damage. One of the candidate materials for structural applications is vanadium and its alloys. Vanadium alloys are attractive since they have a combination of high thermal conductivity and low thermal expansion coefficient and elastic modulus resulting in low thermal stresses. In addition, these alloys are radiation resistant and have excellent compatibility with liquid lithium (which is the coolant in these systems). However, creep and embrittlement are major areas of concern. In my lab, we do both experiments and modeling towards addressing these issues.

If you choose to work on this project, you will have a choice of doing either doing experiments on tailoring the microstructure (by controlling grain size, grain boundary structure or by oxide dispersions) or modeling radiation damage. If you prefer an experimental project, you will be doing a variety of mechanical tests and microstructural studies (SEM/TEM). In the modeling work, you will be doing atomistic simulations, i.e. molecular dynamics and Monte Carlo simulations.

Email me at s.karthikeyan.75@gmail.com for details, or stop by my office (Room A110, Department of Materials Engineering).

Praveen C. Ramamurthy

Charge trapping analysis of organic photovoltaic devices by photoimpedance analysis.

Series resistance is one of the key parameters affecting the performance of organic photovoltaic devices. Several electronic mechanisms arising from different structures within the solar cell can contribute to increasing it. A complete analysis of the impedance response will allow identifying bulk transport resistive circuit elements in the high-frequency part of the spectra. Series resistance dependent on the traps can be evaluated, thus indicating a connection between bulk transport processes and resistive elements. In addition Photo-carrier lifetimes can be measured by impedance spectroscopy of devices under illumination. Photo-generated carriers result in a photo-capacitance that is analyzed as an RC circuit, where C is the photo-capacitance, R is recombination resistance. Here the RC time-constant is the photo-carrier lifetime.

In this project Impedance analysis of various new conjugated molecules will be carried out to determine some of these above properties.

Good reference for this is: Solar Energy Materials & Solar Cells: Volume 94 (2010) Pages 366–375 (available at http://goo.gl/aY2LD7)

Satyam Suwas

Recrystallization mechanisms in high strain hardening systems

In this project, different materials exhibiting twinning and shear banding leading to high strain hardening will be studied. The materials like Nickel-alloys, Titanium alloys and Austenitic steels will subjected to recrystallization after large deformation, and the consequent evolution of microstructure will be studied by microscopic techniques. The kinetics of recrystallization will be evaluated and correlated with the deformation features present in the material. The possible role of recovery will be examined.

References:

- O Engler, X.W Kong, K Lücke, Recrystallisation textures of particle-containing Al–Cu and Al–Mn single crystals, *Acta Materialia*, *Volume 49, Issue 10*, *13 June 2001*, *Pages 1701-1715*
- D.E. Solas, C.N. Tomé, O. Engler, H.R. Wenk, Deformation and recrystallization of hexagonal metals: modeling and experimental results for zinc, *Acta Materialia*, *Volume 49, Issue 18*, *26 October 2001*, *Pages 3791-3801*
- O. Engler, Recrystallisation textures in copper-manganese alloys, *Acta Materialia*, *Volume 49, Issue 7*, *19 April 2001*, *Pages 1237-1247*
- A. Duckham, O. Engler, R.D. Knutsen, Moderation of the recrystallization texture by nucleation at copper-type shear bands in Al-1Mg, *Acta Materialia*, *Volume 50, Issue 11*, *28 June 2002*, *Pages 2881-2893*

T.A. Abinandanan

Phase Field Modeling of Elastic Stress Effects

Phase field models have emerged in the past two decades as a versatile approach to study evolution of microstructures during processes such as phase transformations, grain growth and sintering. Their primary use so far has been in modeling the thermodynamics of interfaces and the kinetics of their migration. In this project, we will explore the application of this approach to study microstructures involving dislocations.

Abhishek Singh
(2 Projects)

1. 2D materials for new generation device

Two dimensional (2D) materials are the ones, where charge carriers are confined in one spatial direction, giving rise to quantum size effect. These materials have attracted great deal of attention due to their unique properties that are intermediate to bulk and small molecules. After experimental realization of graphene [1], search for other 2D materials lead to the synthesis of boron nitride (BN) [2], transition metal dichalcogenides (TMDs) [3], transition metal oxides (MO_2) and silicene, to name a few. All of these materials exhibit different electronic and transport properties and are very promising for nano devices such as nano-electromechanical-systems (NEMS), field effect transistors (FETs), sensors, hydrogen storage, thermoelectric, nano photonics and many more. 2D materials can be used as building blocks for other dimensional materials, e.g., graphene is the mother of all the graphitic nano materials: can be wrapped up to produce 0D fullerene or rolled into 1D nanotube structure or stacked to give rise to 3D graphite. Understanding various properties such as structural, transport, electronic and vibrational properties of these materials is very important for device application. Attempts have been made to modulate their properties by doping, functionalization, applying electric fields, applying pressure, cutting into ribbons or flakes, introducing defects and forming hybrid structures [4-6]. The goal of this project is to explore some recently discovered 2D materials such as silicene, phosphorene as well as some pre-discovered materials such as BN, TMDs and graphene for various applications using first principles based density functional theory (DFT).

Reference:

[1] Novoselov, K. S. et al. *Science* 306, 666–669 (2004).

[2] Pacile´, D., Meyer, J. C., Girit, c. O. & Zettl, A. *Appl. Phys. Lett.* 92, 133107 (2008).

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[5] Yue, Q. et al. *J. Phys.: Condens. Matter* 24, 335501 (2012).

[6] Pan, H. & Zhang, Y.-W. *J. Phys. Chem. C* 116, 11752–11757 (2012).

2. Computational modeling of high ZT thermoelectric

Need to convert the waste heat energy into electricity have fueled the search for a new class of thermoelectric materials. The direct energy conversion between heat and electricity based on thermoelectric effects without moving parts is very attractive for many applications in energy harvesting and heat pumping [1,2,3]. A thermoelectric material's capability of converting heat into electricity is quantified by the figure of merit, $ZT=(S^2\sigma T)/\kappa$, Where, S, σ, T, and κ are Thermopower (Seebeck coefficient), electrical conductivity, temperature and thermal conductivity, respectively. The thermal conductivity has contributions from both electrons (κ_e) as well as phonons (κ_l). The quantity ($S^2\sigma$) is often termed as power factor of a thermoelectric material and is the key to achieving high performance. The power factor is defined as the ability of a material to produce useful electrical power at a given temperature difference. The large power factor is an indicative of better thermoelectric performance. The challenge to model high ZT thermoelectric materials lies in achieving simultaneously high electrical conductivity (σ), high thermopower (S) and low thermal conductivity (κ) within the same material. As these transport properties depend on interrelated material properties such as electronic structure and scattering of charge carriers (electrons or holes), various parameters need to be optimized to maximize ZT [2,3]. The main aim of the project will be proposing efficient thermoelectric materials with high ZT using a combination of density functional theory and Boltzmann transport theory.

References:

1. Zebarjadi, M., et al., *Perspectives on thermoelectrics: from fundamentals to device applications.* Energy & Environmental Science, 2012. **5**(1): p. 5147-5162.
2. Pei, Y., et al., *Convergence of electronic bands for high performance bulk thermoelectrics.* Nature, 2011. **473**(7345): p. 66-69.
3. Joseph R. Sootsman, et al., New and Old Concepts in Thermoelectric Materials, Angew. Chem. Int. Ed. 2009, 48, p. 8616 – 8639.