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RESEARCH

Fields of Research: Metastable Structures (Nanomaterials, Quasicrystals, Amorphous Materials, Defects & Interfaces in Materials). Tools: Finite Element Method, Transmission Electron Microscopy.

Specific Research Accomplishments

- Proved that r^* for homogeneous nucleation in a solid to solid diffusional transformation is not a cardinal time invariant constant– as had been assumed for over 80 years.
- **Discovered** a new kind of *mechanical equilibrium* of an edge dislocation in a semi-infinite body with surface stress. Introduced the concept of surface stress induced torque on edge dislocations (monopole).
- Introduced *new concepts* like: (i) '*depth sensitive lattice fringe imaging*' in the context of nucleation in thin films and (ii) '*nucleation-free zones*'. Established that surface nucleation can occur akin to that in liquids.
- **Demonstrated** '*liquid like nucleation*' in thin solid films.
- Given a **paradigm shift** in hydrogen storage philosophy via *multi-mode* hydrogen storage in nanocontainers.
- Showed for the **first time** storage of molecular hydrogen in a metal. **Demonstrated** storage of molecular hydrogen at atmospheric pressure and room temperature. Enhanced storage involving a novel mechanism with a *dual catalytic role of Pd*. Novel 'idea' to use Sieverts apparatus for 'molecular spectroscopy'.
- Discovered entrapped states of molecular hydrogen at grain boundaries.
- Demonstrated Poisson Effect Driven Anomalous Lattice Expansion in Metal Nanoshells. **Discovered** lattice expansion due to purely surface stress effects in a metallic system.
- Developed a **new** two-scale technique for the *simulation of surface stress*, giving life to Shuttleworth's classic idea from 1949 (which lay dormant for more than 60 years).
- **Discovered** the concept of Orientational High Entropy Alloys.
- Proposed a new Geometrical Parameter for the Formation of Disordered Solid Solutions.
- Simulated the stress state of an *entire multilayer epitaxial device* for the **first time**, taking into account stresses originating from thermal, epitaxial, low angle grain boundaries (threading dislocations) and interfacial misfit edge dislocations.
- **Discovered** material-structures with extended regimes of *negative, zero and positive stiffness*. Showed that there can exist *metastable states of negative stiffness*, along with *unstable states of positive stiffness*. (*these concepts have been considered impossible traditionally*).
- Developed a **new** technique for the determination of coherent to semi-coherent transition in nanoscale precipitates using finite element method. **Discovered** that there can be *two stable regimes* for coherent precipitates. **Computationally and experimentally** showed that the *coherent state can be stabilized* purely by size effects. Considering the tangential stability of an interfacial loop, introduced the concept of a new critical size (r_c).
- Considered the stability of two misfit dislocations for the **first time** and showed they can be stabilized above a critical size of the precipitate (r^{**}). **Defined and computed** a new critical size r_2^{**} , above which an interface with two dislocation loops is *stable* compared to coherent or 'single loop' state.
- Using the example of a plate with an edge dislocation **discovered** a new class of materials: the "*Zero Stiffness Material-Structures*". Introduced a **new** concept of "*Reversible Plastic Deformation due to Elasticity*".
- Giving a **new definition** to the concept of image forces on an edge dislocation; developed **new** a technique to compute image forces in deformable bodies (*without use of images*) → **discovery** that 'image forces' can be attractive (but highly altered in direction and magnitude), *zero or even repulsive (this radically alters the concept of image forces held for about 60 years)*. Introduced the **new** concept of a *positive image*. *Critical size* for dislocation free nanocrystals was determined using this technique.

- **Important proof** that edge dislocations can be mechanically 'stable' in a finite crystal. This solves a longstanding problem for *about 60 years*. The transition from stable to unstable domains is studied for the *first time*.
- Developed *four new* transmission electron microscopy techniques (based on Fourier filtering, zero defocus imaging and Fresnel contrast profiling) for the measurement of thickness of *nanometer scale* Intergranular Glassy Films. This work involved hitherto unknown concepts like: *Fourier filtering of Fresnel contrast images, zero-defocus Fresnel images and Fresnel contrast hidden in lattice fringe images*.
- A **new finding** was made during in-situ heating of Lu-Mg doped Si₃N₄ that fast changes to IGF thickness can occur at comparatively low temperatures (<1000°C) under low irradiation doses.
- Simulation of thin film growth and edge dislocations by imposing stress-free strains. A **novel** method was developed to calculate the critical thickness of nanoscale epitaxial films.
- Developed a **new** perspective of understanding the physics behind the critical thickness of metastable epitaxial films based on an *energy density criterion*.

PROJECTS

☐ Sponsored Research (recent)

- "Hydrogen Storage and Delivery System Based on Inexpensive Industrially Scalable Hybrids", ISRO-IITK Space Technology Cell, 23.0 Lakhs. 2 years (2020-22). Co-PI: Kantesh Balani.
- "Energy Storage Platform on Hydrogen (ESPHy)", Technology Mission Division, DST, 9.83 Crores (IITK component: 1.07 Crores). 5 years (2019-24). PC: Pratibha Sharma (IITB).
- "Nanohybrids for Hydrogen Storage", SERB, DST, 54.79 Lakhs, Period: 3 years (2018-2020). Co-Investigators: Prof. Sri Sivakumar, Prof. Prateek Sen.
- "Computational study of the role of elastic anisotropy, surface stress and compositional segregation in Ge-Si coherent heteroepitaxial growth", SERB, DST. 37.69 Lakhs, 3 years (2017-2019). PI: Prof. Madhav Ranganathan.

☐ Institute Consultancy

- "Synthesis, Characterization and Properties of Al-Ti alloys", Gharda Chemicals Ltd., Mumbai, 1.43 Lakhs, Period: 4 months (2016).
- "Defect Investigation of T90 Barrel", ODC Kanpur/Ordnance Factory Board, 8.75 Lakhs, PI: Prof. Nachiketa Tiwari (Total cost: 94.98 Lakhs), Period: 2 years, (2015).
- "Optimization (Sensitivity Analysis) of T72 & T90 Gun Barrel Manufacturing", ODC Kanpur/Ordnance Factory Board, 99.30 Lakhs, Co-investigators: Prof. Kaustubh Kulkarni, Prof. Shashank Shekhar. (submitted).

☐ Teaching

- "Structure of Materials", Video Course, National Programme on Technology Enhanced Learning (NPTEL), NMEICT, MHRD, Period: 2 Years, 2013.
- "Nanostructures and Nanomaterials: Characterization and Properties", Video Course, National Programme on Technology Enhanced Learning (NPTEL), NMEICT, MHRD, Period: 2 Years, Co-instructor: Dr. Kantesh Balani, 2013.
- "E-book on materials science and engineering", National Mission On Education through Information and Communication Technology, MHRD, 32.21 Lakhs, Period: 1 year, Co-investigator: Dr. Kantesh Balani, 2011.

PUBLICATIONS (recent)

1. "Size reducing rupture during "growth" of LnF₃ (Ln = La, Lu, Y) nanocrystals due to cogeneration of structure and stress"
Debadrita Bhattacharya, Sayantan Sasmal, Ganesh Iyer, Sulay Saha, Anandh Subramaniam, Raj Ganesh Pala, Sri Sivakumar,
Crystal Growth & Design, **21**, p.94, 2021.
2. "Cross-sectional TEM investigation of Mg-LaNi₅-Soot hybrids for hydrogen storage"
Mohammad Faisal, Kantesh Balani and Anandh Subramaniam,
International Journal of Hydrogen Energy, **46**, p.5507, 2021.

3. "Enhanced Reversible Hydrogen Storage in Palladium Hollow Spheres"
Flamina Amaladasse, Anshul Gupta, Suboohi Shervani, Sri Sivakumar, Kantesh Balani and Anandh Subramaniam,
Particulate Science and Technology, **39**, p.617, 2021.
4. "Design of Iso-material Heterostructures of TiO₂ via seed mediated growth and arrested phase transitions"
Deb Sankar De, Dilip Kumar Behara, Sulay Saha, Arun Kumar, Anandh Subramaniam, Sri Sivakumar, and Raj Ganesh S. Pala,
Physical Chemistry Chemical Physics, **22**, p.25366, 2020.
5. "Thermodynamic and Microstructural Basis for the Fast Hydrogenation Kinetics in Mg-Mg₂Ni-carbon hybrids"
Anshul Gupta, Mohammad Faisal Suboohi Shervani, Kantesh Balani, and Anandh Subramaniam,
International Journal of Hydrogen Energy, **45**, p. 11632, 2020.
6. "Triggered Nanoexplosions of Pd Hollow Spheres"
Suboohi Shervani, Anshul Gupta, Sri Sivakumar, Kantesh Balani, and Anandh Subramaniam,
Journal of Nanoscience and Nanotechnology, **20**, p.1941, 2020.
7. "Hybrid Hollow Structures for Hydrogen Storage"
Anshul Gupta, Suboohi Shervani, Sri Sivakumar, Kantesh Balani, and Anandh Subramaniam,
International Journal of Hydrogen Energy, **45**, p.24076, 2020.
8. "Enhanced Reversible Hydrogen Storage in Nickel Nano Hollow Spheres"
Anshul Gupta, Suboohi Shervani, Flamina Amaladasse, Sri Sivakumar, Kantesh Balani, and Anandh Subramaniam,
International Journal of Hydrogen Energy, **44**, p.22032, 2019.
9. "Phase stability and conductivity in the pseudo ternary system of xYb₂O₃-(12-x)Sc₂O₃-88ZrO₂ (0 ≤ x ≤ 5)"
Vandana Shukla, Kantesh Balani, Anandh Subramaniam, Shobit Omar,
Solid State Ionics, **332**, p.93, 2019.
10. "A critical analysis of the X-ray diffraction intensities in concentrated multicomponent alloys"
Rameshwari Naorem, Anshul Gupta, Sukriti Mantri, Gurjyot Sethi, K.V. Mani Krishna, Raja Pala, Kantesh Balani, Anandh Subramaniam
International Journal of Materials Research, **110**, p.393, 2019.

Books (recent)

1. "**Interplay of Stresses, Interfaces and Nanoscale Effects: TEM Investigations**"
Anandh Subramaniam, R.M. Raghavendra and Ganesh Iyer, Arun Kumar
Chapter in *IITK Directions*, Springer, New York, 2022.
2. "**Understanding Disordered Multicomponent Solid Solutions or High Entropy Alloys using X-Ray Diffraction**"
Anandh Subramaniam, Rameshwari Naorem, Anshul Gupta, Sukriti Mantri, K.V. Mani Krishna and Kantesh Balani
Chapter in *High Entropy Alloys: Innovations, Advances and Applications* (Ed: T.S. Srivatsan) Springer, New York, 2020.
3. "**Gases in Nanocontainers**"
Anandh Subramaniam, Suboohi Shervani, Anshul Gupta and Kantesh Balani
Chapter in *Smart Nanocontainers: Fundamentals and Emerging Applications* (Ed: Phuong Nguyen Tri, On Do-Trong, Tuan Anh Nguyen), Chapter-30, Elsevier, 2018. ISBN: 978-0-12-816770-0.

PATENTS

- "Hydrogen Storage in Magnesium based hybrids Using Accumulative Roll Bonding",
Mohammad Faisal, Anshul Gupta, Suboohi Shervani, Kantesh Balani and Anandh Subramaniam,
Patent Pending, Indian Patent Office, January 15, 2014, 119/DEL/2014.