Analytical Model for Gaussian Traps in Organic Thin-Film Transistor—The Application of DEVSIM

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Abstract ID: 10095
: ThinFilms2024
Symposium: 6. Materials Simulation, Design & AI (MSD)
Keywords: Gaussian energy level distribution, TCAD, organic semiconductors, trap states

Currently, the numerical simulation method of semiconductor electronic devices (which is called Technology Computer Aided Design: TCAD) has played a pivotal role in the semiconductor industry. However, the internal core code of commercial products could not be opened to the public, which makes it hard to understand the working details. So, researchers can’t develop their new physical models based on their practical problems. Fortunately, many open-source TCAD tools provide a flexible solution. In this work, we will use the open-source TCAD tool Devsim[1,2] as the core analysis tool to demonstrate its efficiency in defect state analysis for organic semiconductors.

In organic semiconductors, the total density of trap states is much lower than the total density of energy states of the highest occupied molecular orbit (HOMOs) and lowest unoccupied orbits(LUMOs), so Gaussian distribution[3,4] is a better choice to represent it. In this case, our work will present a novel method to calculate the interaction of charges between various Gaussian distribution energy levels of organic semiconductors. This method is based on the Fermi-Dirac statistical distribution and Gaussian energy level distribution function of electrons and uses Miller-Brahm's formula[5] to calculate the generation and recombination rates of trapped charges. To verify the correctness of this model, this work prepared organic field-effect transistors (OFETs) with (DPP-DTT)[6] as the semiconductor layer and then analyzed the transition process between donor-like trap states (DLTs) and the HOMO energy level in the device. Specifically, this article uses self-developed open-source TCAD tools based on the finite volume method DEVSIM[1,2] to build and solve discrete equations. The final analysis results show that this method can perfectly simulate the electrical characteristics of OFETs, and can accurately explain electrical characteristic parameters such as threshold voltage drift of transfer characteristics curves, subthreshold swing changes, and residual trapped charge density.

Density Functional Theory Investigations on the Influence of Substituents and Solvents on Dynamic Covalent Bonds

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Abstract ID: 10246
: ThinFilms2024
Symposium: 6. Materials Simulation, Design & AI (MSD)
Keywords: Recyclable Plastics; Vitrimer; Dynamic Covalent Bonds; Anhydride Exchange

Plastics are widely used in domestic and industrial applications in modern society. However, their cradle-to-grave life cycles are currently extremely linear. Of the 370 million metric tonnes of plastics produced worldwide, only less than 10% is presently recycled, with the vast majority relegated to landfills or incinerated after use. Recycling efforts are predominantly limited to mechanical recycling, which is hampered by the gradual deterioration of material performance that inevitably imposes a finite recyclable lifetime. With the urgent need to reduce the carbon footprint in the near future, the development of new circular plastics built on infinitely recyclable polymers is essential to recapture material values and minimize waste generation. Vitrimers comprising dynamic covalent bonds are the potential circular plastics under research. However, the selection of dynamic covalent bonds for a particular polymer is still by trial and error and is costly and time-consuming. In addition, the bond exchange mechanisms of many dynamic covalent bonds are not fully understood. Furthermore, the bond exchange rates in small molecules and in vitrimers are sometimes very different.

In this work, we use density functional theory (DFT) calculations to study the bond exchange mechanism of anhydride dynamic covalent bonds. The activation energy calculated for model compounds is consistent with the experimental measurement. We further calculate the activation energies for butanoic anhydride with a list of either electron donating or withdrawing substituents, as well as the activation energies in three solvents with low, medium, and high dielectric constants. The details of the approaches and results will be presented and discussed.

Effect of Al and Ca on the interaction between the BaZrO3 crucible and the Ni-based superalloy

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Abstract ID: 10051
: ThinFilms2024
Symposium: 6. Materials Simulation, Design & AI (MSD)
Keywords: BaZrO3 crucible; Ni-based superalloy; Interaction; Thermodynamic calculation

Vacuum induction melting (VIM) metallurgy with a crucible is known to produce Ni-based superalloys. However, oxygen contamination is easily introduced by the crucible. Al and Ca were the common purifying agents for the preparation of the superalloys. This contribution investigated their presence on the effect of the interaction between the alloy melt and the $BaZrO_3$ crucible. The results show that Al addition could react with the dissolved O from the alloy melt, resulting in the formation of Al_2O_3. Then Al_2O_3 reacted with the $BaZrO_3$ crucible, resulting in the formation of a dense Ba-Al-O phase layer with ~10 μm thickness. After adding Al and Ca, no Ba-Al-O phase layer appeared except for a loose CaO layer with ~50 μm thickness. The CaO layer was formed from the direct reaction of Ca addition and the $BaZrO_3$ crucible. The elements Al and Ca were both chemically aggressive to crucibles. Therefore, the content of Al and Ca in the melt should be reasonably controlled when using the $BaZrO_3$ crucible to smelt superalloys. This study offers effective theoretical support for the subsequent preparation of high-purity Ni-based superalloys.

Electrochemical Energy Storage Materials Calculation and Design Siqi Shi

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Abstract ID: 10424
: ThinFilms2024
Symposium: 6. Materials Simulation, Design & AI (MSD)
Keywords: Electrochemical energy storage materials; Multiscale calculations; Machine learning; Database

The key to developing electrochemical energy storage systems such as lithium-ion and sodium-ion batteries lies in materials. The traditional approach to developing new materials is trial and error. It often takes more than ten years to discover and apply new materials using this method, and it is difficult to meet the industry's requirements for higher-performance electrochemical energy storage systems. In this regard, we specialize in establishing a novel research paradigm of structure-performance relationships that cross-integrates calculation, data and experiment, to promote the design of novel electrochemical energy storage materials with long lifetime, high specific power density and high specific energy density. This report will focus on introducing the main progress in this area in recent years based on some work carried out by us and my partners, including: 1) Developing an energy storage materials design platform that mutualistically integrates key algorithm, data and knowledge modules, which has been applied in the electrolyte formula optimization for 37 Ah and other batteries of Contemporary Amperex Technology Co., Limited (CATL), increasing the lifetimes of these batteries by up to 30%. 2) Finding the correlated migration effect of heterogeneous ions and establishing a quantitative model, expanding the methodology of cathode design and electrolyte modification, to guide the synthesis of a NASICON-structured solid-state electrolyte with a Na+ conductivity as high as 5.27 mS/cm at room temperature. 3) Proposing the ligand field stacking topological strategy and the p-type alloying strategy to regulate structural and electronic properties of cathodes, to guide the design of manganese-based composite cathode with high specific power density and light-element carbon-based cathode with 1380 Wh/kg energy density, and the synthesis of intercalation-type Li-free cathode with 554 Wh/kg energy density. Finally, we provide an outlook on the role of cross-scale computing in the development of new materials and systems for electrochemical energy storage.

From Data to Device: Leveraging AI to Overcome Optimization Challenges

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Abstract ID: 10299
: ThinFilms2024
Symposium: 6. Materials Simulation, Design & AI (MSD)
Keywords: , Adaptive Experimentation, Artificial Intelligence

In the rapidly evolving field of thin film technology, the journey from data to device is fraught with complexity. Optimizing thin film properties for cutting-edge applications requires navigating a multidimensional landscape of materials characteristics and process parameters. Traditional experimental approaches, while methodical, often fall short in efficiency and effectiveness, leading to prolonged development cycles and escalated costs. This talk introduces an innovative strategy that leverages artificial intelligence (AI) to overcome these optimization challenges: *Adaptive Experimentation*.

> "***Not all experiments are equally useful.***"

Adaptive Experimentation integrates real-time data analysis to prioritize experiments that yield the most informative results. The core of the method lies in its ability to learn and adapt. Each experiment becomes a stepping stone, guiding subsequent inquiries more intelligently and efficiently. This results in a much faster convergence towards optimal material properties and deposition conditions, not only shortens the development cycle but also accelerates the discovery and optimization of thin films.

Through *DeepVerse*'*s MatCopilot* platform, we will showcase the use of AI-driven methods in accelerating the journey from laboratory research to commercializable devices. By adopting this active approach, researchers and industry professionals can achieve faster material innovation, opening new possibilities in thin film applications across various sectors. This presentation underscores the shift towards a more effective implementation strategy, where progress is achieved and opens new possibilities in thin film applications across various sectors.

Microstructure Evolution and Stability of BaZrO3/Y2O3/Al2O3 Ternary Ceramics Interfaces in Highly Active TiAl Melts

by Lu Mao | Qisheng Feng | Shihua Wang | Xingguang Jin | Haitao Li | Baohua Duan | Dongdong He | Mingrui Lv | Pengyue Gao | Han Miu | Guangyao Chen | Chonghe Li | Shanghai University | Shanghai University | Shanghai University | Shanghai University | Shanghai University | Shanghai University | Shanghai University | Shanghai University | Shanghai University | Shanghai University | Shanghai University | Shanghai University

Abstract ID: 10031
: ThinFilms2024
Symposium: 6. Materials Simulation, Design & AI (MSD)
Keywords: BaZrO3/Y2O3/Al2O3 ternary ceramics; TiAl alloy; Interaction mechanism; Microstructure evolution

$BaZrO_3/Al_2O_3$ dual ceramics presented considerable problems including the dissolution of the low-melting $BaAl_2Si_2O_8$ phase and the volume expansion of ZrO_2 during the cooling process, which led to crack formation at dual ceramics interface after contacted with TiAl melts. Therefore, a Y_2O_3 coating was added at the interface of dual ceramics to prepare novel $BaZrO_3/Y_2O_3/Al_2O_3$ ternary ceramics. The microstructure evolution and stability of ternary ceramics interfaces in highly active TiAl melts were investigated and compared with those of traditional dual ceramics, based on which the corresponding reaction mechanisms of ceramics interfaces were discussed. The results showed that $ZrO_2(Y_2O_3)$, $BaAl_2Si_2O_8$, $BaAl_2O_4$, and $BaAl_{12}O_{19}$ were formed with poor thermodynamic stability at the interface of dual ceramics. And the $Y_3Al_5O_{12}$ phase with high thermodynamic stability and high strength was formed at the interface of ternary ceramics. After that, $Y_3Al_5O_{12}$, $YAlO_3$ and $Y_4Al_2O_9$ phases with high melting point and high thermodynamic stability were formed at the Y_2O_3/Al_2O_3 interface, which could effectively prevent the penetration of TiAl melt into the backup coatings during the interaction experiment. Therefore, the volume fraction of inclusions when using ternary ceramics were much lower than using dual ceramics, making the former promising candidate molds for the high quality directionally solidified of highly active TiAl alloys.

Multiscale Simulation Empowers the Construction of Digital Materials R&D Platform

by Kui Gong | Hongzhiwei Technology Co., LTD

Abstract ID: 10309
: ThinFilms2024
Symposium: 6. Materials Simulation, Design & AI (MSD)
Keywords: Multi-scale simulation, high-throughput computing, material design

Multi-scale simulation is a powerful tool for deeply mining and fully exploiting the value of materials data, and is important for constructing a powerful digital material R&D (research and development) platform. The integration of multi-scale simulation with digital material R&D platform is reshaping the R&D paradigm of materials. It not only enhances the efficiency and quality of material development but also helps to improve material performance, increasing the predictability and specificity of material design. Multi-scale simulation is becoming an essential weapon for new material innovation and a booster for traditional material upgrading.

The report mainly introduces the digital materials R&D (research and development) platform developed by Hongzhiwei and its industrial application cases. The digital platform integrates modules such as intelligent materials database, multi-scale simulation software, high-throughput computing workflow engine, and AI (artificial intelligence) algorithms. Data of the intelligent materials database are from independently controllable sources, and can be combined with AI technology for material screening and performance prediction. The multi-scale simulation tools, when combined with the high-throughput computing workflow engine, can efficiently design and screen materials, helping enterprises reduce costs and increase efficiency. The report will also present successful cases born out of Hongzhiwei's collaboration with leading enterprises in fields such as lithium batteries, chemical industry, alloy and steel industry, and semiconductor industry. These cases include electrolyte screening, polymer performance prediction, alloy material design, and robot scientist development.

Multiscale simulation of vitrimers

by zheng jianwei | Li Nannan | Zhang Xinglong | Anjaiah Nalaparaju | chen qiubo | Michael Sullivan |
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Abstract ID: 10538
: ThinFilms2024
Symposium: 6. Materials Simulation, Design & AI (MSD)
Keywords: DFT, Monte Carlo, dynamic covalent bond, kinetic Monte Carlo, machine learning, mesoscale, molecular dynamics, vitrimer

Thermoset polymers are an important class of high-performance polymers, used in many industrial applications and daily life. Some examples are vulcanized rubber, epoxy, melamine, polyurethane, urea formaldehyde etc. Due to the presence of permanent covalent crosslinks, these materials are impossible to reprocess and difficult to recycle. Therefore, they are one of sources of plastics waste. An Intelligence Brief by PreScouter in 2022 indicated that with approximately 11% of plastic production volume worldwide consisting of thermosets, the development of new recycling solutions for these materials could potentially have a major impact on global efforts to reduce fossil-based plastic waste. Installation of dynamic covalent bond linkages into thermoset polymers could impart these thermoset polymers reprocessability at certain temperature and is a potential solution to produce infinitely-recyclable polymers to recapture material values and minimize waste generation. Such thermoset polymers with dynamic covalent bonds could be called vitrimers. Much progress in vitrimer development has been achieved. However, there are still many problems to be resolved, such as selection of proper dynamic covalent bonds for a given polymer, properties of resulted vitrimers, recyclability and stability etc. In this talk, application of molecular and meso-scale simulation and machine learning in vitrimer field will be reviewed and discussed.

Physics-based AI for Material Design

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Abstract ID: 10404
: ThinFilms2024
Symposium: 6. Materials Simulation, Design & AI (MSD)
Keywords: Generative AI, Inverse Modeling, Physcics-based AI

Physics-based AI, defined as a branch of artificial intelligence that incorporates principles and models from physics, revolutionizes material design by facilitating faster and more accurate optimization. This talk explores the synergies between traditional inverse modeling approaches, such as genetic algorithms and particle swarm optimization, and Physics-based AI techniques, demonstrating their combined effectiveness in accelerating material design processes. By harnessing the power of Physics-based AI, researchers can achieve enhanced understanding and predictive capabilities, enabling the rapid exploration of vast design spaces to discover novel materials with tailored properties. Additionally, the incorporation of Physics-based generative AI holds promise in further accelerating material design by enabling the automated generation of candidate materials based on desired specifications. In this talk, we will share some of our current research on Physics-based AI for material design.

Plastic Deformation and Tribological Properties of Cu/Ta Nanoscale Multilayer Films by Molecular Dynamics Simulations

by Junqin Shi | Northwestern Polytechnical University

Abstract ID: 10281
: ThinFilms2024
Symposium: 6. Materials Simulation, Design & AI (MSD)
Keywords: Cu/Ta Nanoscale Multilayer Film; Plastic Deformation; Tribological Properties; Molecular Dynamics Simulations

Nanoscale multilayer materials (NMMs) are widely used in mechanical processing, aerospace, navigation, and microelectronic devices fields. Cu/Ta NMMs plays an important role in the manufacture of semiconductors and superconductors, and herein the effects of interface, single layer thickness, orientation and other factors on the plastic deformation and friction and wear properties of Cu/Ta NMMs are clarified by molecular dynamics simulations. The results show that the plastic deformation mechanism of Cu/Ta NMMs is determined by the intrinsic properties of single layer and interface properties, revealing the presence of two critical thicknesses. The nanoscratching tests indicate that Cu/Ta interface absorbing dislocations and preventing their propagation is different from the Ta/Cu interface, and the friction and wear properties of Cu/Ta multilayers are significantly improved with the decrease of monolayer thickness. Furthermore, the Cu100-xNix/Ta multilayers with addition of Ni element were established to reveal the effect of different alloying degrees on hardness and wear resistance. The alloying with can effectively enhance the hardness and wear resistance of Cu/Ta multilayers, and the content of Ni has a great influence on the hardness and wear resistance of Cu/Ta multilayers. This work provides a reference for the design of Cu/Ta NMMs with excellent friction and wear properties, and Cu/Ta NMMs with high hardness and wear resistance are designed by alloying method and their mechanical and tribological properties are strengthened.

Keywords: Cu/Ta Nanoscale Multilayer Film; Plastic Deformation; Tribological Properties; Molecular Dynamics Simulations

Thermodynamic Description of Polycrystalline Phase Segregation in Dual-doped CsxRb1-xPb(BryI1-y)3 Film System

by Han Miao | Qisheng Feng | Shihua Wang | Jianzhou Huang | Lu Mao | Kun Wang | Chonghe Li | Shanghai University | Shanghai University | Shanghai University | Shanghai University | Shanghai University | Polytechnique Montréal | Shanghai University

Abstract ID: 10028
: ThinFilms2024
Symposium: 6. Materials Simulation, Design & AI (MSD)
Keywords: Calphad, DFT, Perovskite, Phase segregation, Thermodynamic description

As an ideal wide bandgap material, $Cs_xRb_{1-x}Pb(Br_yI_{1-y})_3$ has been extensively employed in the top light-absorbing film of triple-junction perovskite solar cells, achieving efficiencies surpassing 24%. However, because of the lack of theoretical study on thermodynamics, the conventional dual-doping experiment induces undesirable polycrystalline phase segregation. Through density functional theory (DFT) and the Calphad method, we explore the inherent thermodynamic mechanism governing the compositional changes and polycrystalline phase segregation in $Cs_xRb_{1-x}Pb(Br_yI_{1-y})_3$. Utilizing the Compound Energy Formalism (CEF) model and reciprocal system in the Calphad method, we identify specific component regions ($0.89 < x_{Cs} < 1$, $0.5 < y_{Br} < 0.85$) conducive to maintaining the cubic structure at room temperature through controlled A-site and X-site manipulation, thereby circumventing detrimental polycrystalline phase segregation.

Thermomechanical properties of shape memory polymer IBOA-PEGDA system by molecular dynamics simulation

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Abstract ID: 10313
: ThinFilms2024
Symposium: 6. Materials Simulation, Design & AI (MSD)
Keywords: Crosslinked polymers, Molecular dynamics simulation, Shape memory polymers

Shape memory polymers (SMPs) have proven their value in various fields such as medicine, robotics, and aerospace applications due to shape-recovering to the initial shape by stimulation. In general, SMPs are subjected to thermomechanical cycles involving heating, deforming, and cooling to store stress. Subsequently, re-heating is employed to release stress and recover to its original shape. Consequently, it is important to understand the thermomechanical properties such as glass transition temperature and temperature-dependent modulus within the SMP cycle for the desirable utilization of SMPs.

Thermomechanical properties of SMPs, especially those of crosslinked thermoset polymers, vary significantly depending on the nature of the crosslinker such as crosslinker structure, crosslinker concentration, and crosslinking concentration. Many experiment-based studies have been conducted to understand the thermomechanical properties of SMP. However, experimental optimization of the formulation is a time-consuming and expensive process, particularly due to the limited search space.

To address these issues, we utilize an approach merging automated crosslinking workflow with molecular dynamics (MD) simulation, offering a cost-efficient way to explore extensive screening spaces. We take the isobornyl acrylate-polyethylene glycol diacrylate (IBOA-PEGDA) system as an example, which has not been reported despite being promising SMP. IBOA is a widely used photocurable monomer with a high glass transition temperature and strong shape-recovering stress, attributed to the sizable side groups that do not participate in crosslinking. As a crosslinker, PEGDA is often used in crosslinked polymer systems. We create various crosslinked IBOA-PEGDA molecular models by adjusting the crosslinker concentration, chain length, and crosslinking density, then compute the glass transition temperature and modulus via MD simulation. This presentation will cover how crosslinking parameters influence the glass transition temperature and modulus, compare simulation outcomes with experimental data, and display the crosslinked IBOA-PEGDA's morphology. This approach provides valuable insights into the molecular nature of SMPs, thereby accelerating material development.