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LL13-MatModelRadDetect-PD2Jf Final Report: Materials Modeling for High-Performance Radiation Detectors

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I. INTRODUCTION

The aims of this project are to enable rational materials design for select high-payoff challenges in radiation detection materials by using state-of-the-art predictive atomistic modeling techniques. Three specific high-impact challenges are addressed: (i) design and optimization of electrical contact stacks for TlBr detectors to stabilize temporal response at room-temperature; (ii) identification of chemical design principles of host glass materials for large-volume, low-cost, high-performance glass scintillators; and (iii) determination of the electrical impacts of dislocation networks in $\mathrm{Cd}_{1-x}\mathrm{Zn}_x\mathrm{Te}$ (CZT) that limit its performance and usable single-crystal volume. The specific goals are to establish design and process strategies to achieve improved materials for high performance detectors.

Each of the major tasks is discussed below in three sections, which include the goals for the task and a summary of the major results, followed by a listing of publications that contain the full details, including details of the methodologies used. The appendix lists 12 conference presentations given for this project, including 1 invited talk and 1 invited poster.

II. TlBr CONTACT MATERIALS

A. Overview and Goals

TlBr detectors show great promise for high-resolution room-temperature gamma detectors, but temporal decay of their performance (*e.g.*, energy resolution) have stymied practical implementation.[1–5] Choice of contact metal and the nature of materials interfaces near the contact play significant roles in detector instability.[6–9] The goals of the present project are to elucidate the effects of the metal contacts, from various points of view: (i) the impact of possible metal impurity contamination into the active material from the contact layer, (ii) the role of heterostructures from interphases formed incidentally or intentionally at the TlBr–metal interface, and (iii) the design principles for engineered heterostructures to maximize detector stability ("longevity"). The effects can be driven by electrochemical effects, which differ at the anode and cathode side of a device. The knowledge gained allows for improved rational design of optimal contact stacks.

B. Major Results

1. *Metal Contacts*

We evaluated the impact of 13 different metals as sources of impurities from both anode and cathode electrodes: Mo, Pt, Pd, Ni, Al, Au, Bi, Cr, Ag, Cu, Ti, In, and Pb. For each metal, we computed the solubility in TlBr, the charge state of the metal as an impurity, the diffusivity, and the association of deep or shallow traps in TlBr (for both electrons and holes), for conditions associated with the anode (Br-rich, low Fermi level) and cathode (Tl-rich, high Fermi level) sides of the device. Metals that introduce deep electron traps in TlBr and that exhibit high solubility and high diffusivity are expected to be particularly detrimental to device longevity, since increasing numbers of electron traps could move through the device during operation, affecting charge collection and also the internal field. In addition, positive charges are attracted to the cathode, while negative charges to the anode. After evaluation of all these factors, Pt, Ni, Pd, and Mo were suggested as the most favorable metals, since these have low solubilities, low diffusivities, low electron trap concentrations, and Pt forms a neutral impurity, which will not drift in the electric field. Of these, Pd has a high solubility, but forms neutral impurities with no traps, while Mo introduces a deep trap but has extremely low solubility and low diffusivity. Aluminum is a particularly poor choice, since it introduces deep traps, is moderately soluble, and fast diffusing. Chromium is predicted to be a possible alternate choice for the anode; although it introduces significant electron traps, the diffusivity is extremely low. These results are consistent with experimental realizations of high-longevity devices using Pt, Ni, and Cr–Ni contacts.

2. *$TlBr_{1-x}Cl_x$ Heterojunction Compound*

Experiments demonstrated that HCl treament of TlBr can produce improved longevity detectors.[6] Our combined experimental and theoretical investigations identified formation of $\mathrm{TlBr}_{1-x}\mathrm{Cl}_x$ on the surface, which provides advantage when inserted between the bulk TlBr and the metal contacts. Detailed electronic structure calculations for the range of alloy compositions from TlBr to TlCl, combined with experimental analysis with X-ray photoemission spectroscopy, was used to map the absolute positions of the conduction and valence bands as a function of composition. We determined that a small conduction band offset of between -0.1 and 0.2 eV relative to TlBr exists for the entire composition range of $\mathrm{TlBr}_{1-x}\mathrm{Cl}_x$, while most of the increase in band gap of TlCl relative to TlBr occurs in the valence band (∼0.5 eV for TlCl). The formation of a graded profile of $\mathrm{TlBr}_{1-x}\mathrm{Cl}_x$ on the surface of TlBr creates a wider band gap interphase between the bulk and the metal contact that can prevent migration of both vacancies and impurities (the energy barrier for diffusion is higher in TlCl than TlBr) without introducing a barrier for electron transport. In addition, the valence band offset blocks hole transport, which can mitigate the formation of excess (charged) vacancies at the contact interface by providing charge compensation. These results further suggest that addition heterostructure engineering of the contact stack can be beneficial, following the design rules implied by $\mathrm{TlBr}_{1-x}\mathrm{Cl}_x$.

3. *Contact Metals for Engineered Interphase Compounds*

Following on the principle of using HCl treatment to generate a contact interphase compound between the bulk TlBr and metal contact, we explored the selection of specific contact metals to promote formation of interphase compounds with TlBr and/or TlCl/$\mathrm{TlBr}_{1-x}\mathrm{Cl}_x$by diffusion of metal and chemical reaction with the semiconductor. We focused primarily on compounds formed with either Pt or Au.

First we computed the thermodynamic stability of different possible phases of Pt- and Au-containing compounds with TlBr(Cl) for stoichiometric, Tl-rich, and halide-rich conditions, which correspond to pristine material, material evolved under the cathode, and material evolved under the anode, respectively. We found a number of thermodynamically stable interphase compounds, particularly for halide-rich conditions. In particular, depending on the degree of excess halide, the following compounds were found to be stable: $\mathrm{PtBr(Cl)}_3$, $\mathrm{Tl_2PtBr(Cl)}_6$, $\mathrm{AuBr(Cl)}_3$, $\mathrm{TlAuBr(Cl)}_4$. The $\mathrm{Tl_2PtBr_6}$ compound is especially interesting because it has a similar band gap as TlBr and the band edges are nearly aligned, so charge transport is not affected; however, migration energy barriers for vacancies are at least double in this compound compared to TlBr or TlCl, so it forms a very good barrier layer for vacancies. This effect acts predominantly at the anode side, which becomes significantly halide-rich after initial operation of the device. These predictions were validated with experiments that used accelerated testing and cross-sectional transmission electron microscopy to observe growth of the interphase compound $\mathrm{Tl_2Pt(Br,Cl)}_6$ between TlBrCl and Pt contacts, as increasing current (vacancy flux) was run through the device in the dark. Devices fabricated with HCl surface treatment and Pt contacts showed among the best longevity of any devices fabricated. Our chemical analysis also revealed the presence of $\mathrm{Tl(Br,Cl)}_2$ secondary phases when the surface becomes extremely halide-rich; the significance of this phase was not determined. Finally, we noted improved operation of devices as long as these interphases formed continuous layers; after extreme vacancy current flow, a porous layer was observed to form, which impeded detector performance due to poor electrical transport.

C. Publications/Deliverables

1. K.G. Ray, J.B. Varley, and V. Lordi, “Chemical Thermodynamics of TlBr-Metal Interfaces,” *LLNL Technical Report* LLNL-TR-677657 (2015).
2. J.B. Varley, K.G. Ray, and V. Lordi, “Heterostructure Effects on Device Stability of TlBr Radiation Detectors,” *LLNL Technical Report* LLNL-TR-677665 (2015).
3. K.G. Ray, C.R. Leão, and V. Lordi, “The role of metal contacts in the degradation of TlBr radiation detectors,” *to be published*; LLNL-JRNL-739134-DRAFT.
4. J.B. Varley, A.M. Conway, L.F. Voss, E. Swanberg, R.T. Graff, R.J. Nikolic, S.A. Payne, V. Lordi, and A.J. Nelson, “Effect of chlorination on the TlBr band gap for improved room temperature radiation detectors,” *Physica Status Solidi B* **252**, 1266 (2015); LLNL-JRNL-661938. ***[Back Cover article]***
5. K.G. Ray, J.B. Varley, Z. Dai, N.E. Teslich, J. McKeown, A.M. Conway, A.J. Nelson, L.F. Voss, E.L. Swanberg, R.T. Graff, S.A. Payne, and V. Lordi, “Combined computational and electron microscopy study of compounds formed between TlBr and metallic contacts,” *to be published*; LLNL-JRNL-713003-DRAFT.

III. GLASS SCINTILLATOR HOST MATERIALS

A. Overview and Goals

Glass scintillators may hold great promise for low-cost, large-volume, formable detectors; however, the light yield and energy resolution of current materials have been more than an order of magnitude worse than crystalline scintillators and far from the theoretical limits. Fundamental understanding of carrier transport and limits on activator loading of different glass hosts is lacking and is essential to designing high-performance glass scintillators.

Rational design of improved glass hosts for bright scintillators requires gaining knowledge of the correlation of glass chemistry with atomic structure and charge transport. The goals of this task are to use atomistic simulations (molecular dynamics and density functional theory-based electronic structure calculations) to gain fundamental insight into the correlations between composition, structure, electronic states, and carrier transport in glass materials, as potential high-performing hosts for scintillators. The results shed light on factors affecting composition and processing of glass scintillator materials for maximum charge transport and optimal dopant activation. Silicate- and phosphate-based materials of various compositions are studied are model systems.

B. Major Results

1. Silica and Sodium Silicate Glasses

We studied several different host glass compositions based on silica (SiO_2), as benchmark cases. Pure silica is a very well understood material, and modestly-performing scintillators have been fabricated from Ce-doped silica.[10] Sodium silicate $[(Na_2O)_x(SiO_2)_{1-x}]$ glasses doped with Ce have also been tested as scintillators and found not to scintillate.[11] We analyzed two compositions of sodium silicate glass (x = 0.2 and 0.3) and compared to silica to understand the origin of scintillation quenching in the sodium-containing materials.

We used a computational melt-quench-anneal technique to generate representative atomic structural models of each glass composition of interest. To better sample the heterogeneity of the amorphous structures using a relatively small number of atoms ($\sim$ hundreds), we took about 30 structures from each melt and performed independent quenches, then averaged the results over all the sampled structures. Semi-empirical molecular dynamics was used for the melt-quench-anneal process, while final structures were further relaxed with density functional theory to study the electronic properties. Each glass composition was analyzed to characterize its atomic-structural features, in particular statistics of interatomic distances (structure factors), angles, ring sizes, and so-called “Q-numbers,” which measure the local number of non-bridging oxygen atoms in silica-based materials; this latter feature was found to critically determine the carrier transport properties of the glass, most important for efficient scintillation.

The analyses produced a detailed understanding of the microscopic structural nature of carrier traps in these glasses leading to poorer carrier transport for the sodium-containing materials. Sodium is a network-modifying additive that increases the number of non-bridging oxygen atoms, denoted by a higher fraction of low Q-number local structures (for these tetrahedral materials, Q-numbers range from Q^0 to Q^4). We developed and applied a novel analysis method to map the local atomic structures onto the electronic states controlling transport in the material. Specifically, we decomposed the electronic density of states into contributions from each local atomic environment characterized by the different Q-numbers, then analyzed the nature of carrier transport for each mapped state via "inverse participation ratio" analysis. The result is a quantitative graphical analysis of the mobility edges, along with the density of carrier traps near the band edges and in the band tails, labeled by the associated local atomic structures. This technique is a novel way to explore the electronic transport properties of glass materials, which are usually considered insulators.

In the comparison of silica with $(Na_2O)_{0.2}(SiO_2)_{0.8}$ and $(Na_2O)_{0.3}(SiO_2)_{0.7}$, we found that increased Na content leads to a prominent increase in electronic density of states near the top of the valence band. The large majority of these states were found to be associated with low-Q-number (Q^1 and Q^2) local atomic structures which highly localize charge. These structures create a high density of hole traps, which degrade the carrier transport in sodium silicate so that photogenerated holes cannot reach the Ce activators to emit light for scintillation.

This detailed view of the structure–property relationship suggests target glass structures for maximal performance. In the case of (sodium) silicates, a more perfect local structure similar to that of crystalline quartz (all Q^4 local structures) is the optimal material, but silica is only a modestly-performing scintillator host. Thus, with this knowledge gained, additional glass chemistries must be explored to find potentially high-performing glass scintillator hosts.

2. *Zinc-Oxide Phosphate Glasses*

Zinc-oxide phosphate $[(ZnO)_x(P_2O_5)_{1-x}]$ glasses doped with Sn have shown some promise recently as phosphors or scintillators,[12–19] with the added advantage of being rare earth-free. We constructed atomistic models for two different compositions of $(ZnO)_x(P_2O_5)_{1-x}$ with $x = 0.6$ and 0.7, using similar procedures as described above for the silica-based glasses, and examined the relationships between local structural, electronic, and optical properties associated with scintillation performance. We found the structures to consist of nearly ideal tetrahedral PO_4 unit and largely distorted ZnO_4 and ZnO_5 units. The concentration of ZnO_5 units is calculated to increase and exceed that of ZnO_4 as the amount of ZnO in the glass is increased. Also, the concentration of terminal oxygen atoms shared by two Zn neighbors is largely increased for the $x = 0.7$ glass compared to $x = 0.6$. In addition, Q^1 and Q^2 structures (where here Q^n refers to structures containing n bridging oxygen atoms on PO_4 tetrahedra) are dominant for the $x = 0.6$ glass, while Q^0 and Q^1 prevail for the $x = 0.7$ glass.

When doped with Sn, various Sn coordination geometries are found, with trigonal pyramidal SnO_3 and largely distorted pyramidal SnO_4 configurations being dominant and a small fraction of two-fold and five-fold coordinated Sn configurations also present. Two-fold coordinated Sn are found to exhibit slightly smaller optical transition energy than three-fold and four-fold coordinated Sn. However, local variations of the Sn coordination structures in the glass broaden the excitation bands, which lie around 5.4 eV for all the different Sn configurations; the broadening is generally larger than the differences in excitation energies for local environments with different coordination number, leading to an intrinsically broad excitation/emission band in the glass. The results is a fraction of the Sn dopants being effectively inactive, corresponding to those in the tail of the spectral distribution above the band gap of the host.

We can extrapolate these results for $(ZnO)_x(P_2O_5)_{1-x}$:Sn to understand general routes to high performance (bright) glass scintillators based on non-rare-earth dopants. From our analysis of Sn in zinc-oxide phosphates, we found that the electronic structure of the dopant is sensitive to the local coordination environment, with the coordination number grossly affecting the excited state energy level of Sn. The effect of coordination number can possibly deactivate the dopant if the excited state energy is pushed above the host conduction band, which is possible with higher coordination numbers. The overall effect is that certain fractions of dopants with a given coordination number are inactive, increasing with coordination number and dependent on glass composition and density. Maximizing the scintillator performance requires manipulating the glass structure to maximize dopant activation; several routes are suggested (summarized in the next paragraph). In addition, good carrier transport is required for photogenerated carriers to reach the activators; the $(ZnO)_x(P_2O_5)_{1-x}$ system can have good carrier mobilities, because the ZnO base material leads to fairly dispersive bands and a small mobility gap, unlike the sodium-silicate glasses discussed above.

We determined general trends on the path to bright glass scintillators using non-rare earth activators. In general, the energy states of O atoms in the glass are important for determining the activator energy level alignment. The O states are dependent on the ratio of glass former (P_2O_5 in the system studied here) to modifier (ZnO in the system studied here). For ns^2-type activators (post-transition metal, such as Pb, Sn, and Bi), the optical and electronic properties are strongly affected by the coordination environment with neighboring O atoms, since the optical transition occurs in their outermost valence states (from ns^2 to ns^1np^1). One way to control the coordination environment, and thus the activation of the ns^2-type dopant, is by glass composition; in the case of $(ZnO)_x(P_2O_5)_{1-x}$ with $x \sim 0.6 - 0.7$, increasing the ZnO fraction reduces the Sn coordination and increases the number of activated dopants. With lower ZnO fractions, up to 20% of randomly-doped Sn may be inactive. The coordination environment is also sensitive to the glass network density, since the activator dopants have non-bonding lonepair electrons; a more flexible and less dense glass network that facilitates activation of dopants could be achieved with glass additives or negative pressure applied during synthesis. Finally, ns^2-type dopants can easily be oxidized to give ns^0 electronic configuration (*e.g.*, $Sn^{2+} \rightarrow Sn^{4+}$), which is inactive for scintillation; thus, non-oxidizing growth conditions will maximize dopant activation and may be achieved, for example, with Ar atmosphere or addition of S to the glass.

C. Publications/Deliverables

1. N. Adelstein and V. Lordi, “Report: Comparison of Atomic and Electronic Structures of Silica and Sodium Silicate Glasses,” *LLNL Technical Report* LLNL-TR-663696 (2014).

2. N. Adelstein, C. Olson, and V. Lordi, “Hole traps in sodium silicate: first-principles calculations of the mobility edge,” *Journal of Non-Crystalline Solids* **430**, 9–15 (2015); LLNL-JRNL-673719.

3. K.E. Kweon and V. Lordi, “First principles study of the structural, electronic, and optical properties of Sn^{2+}-doped ZnO-P_2O_5 glasses,” submitted to *Journal of Non-Crystalline Solids*; LLNL-JRNL-711877-DRAFT.

IV. Cd(Zn)Te DISLOCATIONS

A. Overview and Goals

$Cd_{1-x}Zn_xTe$ (CZT) is the most mature and highest performing room-temperature gamma radiation detector material, but high-yield growth of large uniform crystals with spectroscopic quality remains problematic, driving up the cost. One of the remaining issues affecting performance is the electrical impact of dislocation networks in the material, namely how dislocations and associated structures capture carriers and reduce their lifetimes. In particular, questions remain about the role of the dislocation cores themselves on carrier capture versus impurities or tellurium precipitates frequently associated with the dislocations, which is extremely challenging to disentangle experimentally.

This project explores the fundamental atomic structures and carrier capture and transport properties of dislocations in CdTe—which is a good model surrogate for the CZT alloy system—as well as their interactions with defects and impurities that may accumulate at the cores and the consequent effects on the electronic properties.

B. Major Results

1. Dislocation Structures, Energetics, and Charge Transport

A number of different types of dislocation in CdTe were explored, including edge, screw, and mixed dislocations. For each dislocation type, various core structures were explored to find the most stable configuration. Also, since CdTe is a compound semiconductor, two core stoichiometries are possible (except for the screw dislocation, which remains stoichiometric), termed Cd-core or Te-core, depending on which element exists in excess at the dislocation core. The dislocations investigated include the $[\bar{1}10]$ screw, $[\bar{1}10]$ edge (various core configurations), 60° mixed perfect glide dislocation, and 30°/90° partial glide dislocations. The 60° glide dislocation is known to be one of the most common dislocations in CdTe; this dislocation can dissociate into pairs of 30° and 90° partials with a stacking fault between them. The $[\bar{1}10]$ screw and $[\bar{1}10]$ edge are also observed in electron microscopy.

Three possible core configurations for the $[\bar{1}10]$ edge were considered, characterized by the number of atoms in ring structures present in the core: 8-core, 4-core, and 5-7-core (the latter contains two rings in the core from strong Cd–Cd or Te–Te dimerization). A Cd-core and Te-core version of each structure was studied. Generally, Te-core and Cd-core dislocations occur in pairs in a CdTe crystal to maintain overall stoichiometry, but for Te-rich material typical of radiation detectors, excess Te-core structures are expected. For the Te-core edge dislocation, the 5-7 structure was found to be most stable, while the 8-core structure is most stable for the Cd-core. Screw dislocations were found to be more stable than all the pure edge dislocations. Electronically, the screw dislocation was found to introduce no gap states. The most favorable Te-core (5-7) exhibits a mid-gap state that actually promotes conduction along the dislocation line. A similar gap state exists for the Cd-core, but is closer to the valence band maximum and more prone to trap charge.

For the 60° dislocations, which are probably the most prevalent, a significant reconstruction along the dislocation line was found that converts the core from metallic character to semiconducting (or gapped) character. The reconstruction involves dimerization along the dislocation line in a "quadruply-periodic" fashion (*i.e.*, involving four unit cells along the dislocation line). The significance of the reconstructions is that they cause localization of charge ("polarons") along the dislocation line, disrupting the conducting channel observed in the pure edge dislocations. The energy barrier to move the polaron along the dislocation line is large (greater than 0.5 eV), which means that charge transport along the 60° dislocations is inhibited. Similar behavior was found for the 30° dislocations, except these partial dislocations introduce mid-gap states that are not present for the 60° perfect dislocations.

The formation of polaronic structures along the 60° and 30° dislocation lines is associated with charge modulation along the dislocations, with alternating regions of localized charge accumulation and depletion (electrons for the Cd-core and holes for the Te-core), to maintain overall charge neutrality of the crystal. This behavior is competitive with global charge transfer from (single-periodic) Cd-cores to Te-cores, which has been suggested previously. However, our calculations find that the intra-core charge modulation accompanied by core reconstruction is energetically much more favorable, by more than 1.0 eV, than inter-core charge transfer. In addition, for off-stoichiometric crystals, the excess of Te-cores implies that the intra-core process must be involved, at least for the unbalanced cores.

2. *Tellurium Clustering at Dislocation Cores*

Previous work[20] suggested a bulk-mechanism for Te nucleation in Cd(Zn)Te involving point defect migration and reactions. Namely, we found that highly mobile Te interstitials react with Cd vacancies to form immobile Te antisite defects, which further react with Te interstitials to form Te clusters (nuclei). In our study of dislocations, we computed the relative stability of point defects in the core of dislocations compared to the bulk crystal, for Te interstitials, Cd vacancies, and Te antisites. We found generally that all point defects are more stable inside a dislocation core than in the bulk crystal, by ∼0.5–2.5 eV, regardless of type of dislocation or core stoichiometry. Differences in the degree of stability in a core depend on the type of defect and core stoichiometry (*e.g.*, a Cd vacancy is much more stable in a Cd-core than a Te-core), but no defects are found to be less stable in a dislocation core than in the bulk. We also computed the formation energy of the defects as a function of distance away from the core and found a region of stability extending about 5–10 Åfrom the center of the core, implying a region of "capture" for point defects that migrate to a core; since the energy cost of moving a point defect away from the core is so great, once a defect is captured it can only migrate along the dislocation, and then only until another defect is encountered. In addition to capture and binding at the core, some point defects prefer to *form* at the core of dislocations (*i.e.*, have lower absolute formation energy in a core than in the bulk); namely, the Te interstitial prefers to form in Te-core dislocations, while Cd vacancy and Te antisite both prefer to form in Cd-core dislocations.

A mechanism for Te clustering at dislocations associated with point defects was found that is analogous to the mechanism for point defect-mediated Te nucleation in the bulk. At dislocations, rapid flux of Te interstitials from the bulk (or interstitials that formed in the core) have a tendency to cluster, since rapid diffusion along dislocations is only one-dimensional (the energy barrier for Te interstitial migration along a dislocation line is 0.18 eV, similar to the value for diffusion in the bulk, 0.16 eV). In addition, Cd vacancies in dislocations are very mobile (0.26 eV migration barrier, compared to 1.09 eV in the bulk). Small stable clusters of Te that may even extend slightly outside the dislocation core can form when additional Te interstitials arrive. This local enrichment of Te concentration at a dislocation is enhanced by formation of immobile Te antisite defects when a Cd vacancy and Te interstitial interact. The structure of Te clusters in the dislocation core is reminiscent of bulk Te and suggests a mechanism for nucleation and growth of Te precipitates at dislocation cores. Such a process would be consistent with frequently observed Te precipitates decorating dislocations.

C. Publications/Deliverables

1. K.E. Kweon, D. Åberg, Vincenzo Lordi, "First-principles study of atomic and electronic structures of 60° perfect and 30°/90° partial glide dislocations in CdTe," *Physical Review B* **93**, 174109 (2016); LLNL-JRNL-677727.
2. K.E. Kweon and V. Lordi, "Behavior of point defects and clustering of Te near the 30° dislocations in CdTe," *to be published*; LLNL-JRNL-739133-DRAFT.

V. APPENDIX: CONFERENCE PRESENTATIONS

Presenting author is noted with an underline.

A. TlBr Contact Materials

1. K.G. Ray, J.B. Varley, C.R. Leao, and V. Lordi, "First Principles Study of Semiconductor-Metal Contact Interactions in TlBr Room Temperature Radiation Detectors," R4D-5, presented at *IEEE NSS/RTSD*, San Diego, October 31–November 7, 2015; LLNL-PRES-678952.
2. K.G. Ray, J.B. Varley, A.M. Conway, A.J. Nelson, L.F. Voss, E.L. Swanberg, R.T. Graff, S.A. Payne, and V. Lordi, "Combined Computational/Experimental Study of Semiconductor-Metal Contact Interfaces in TlBr Radiation Detectors," R16-6, presented at *IEEE NSS/RTSD 2016*, Strasbourg, France, October 29–November 5; LLNL-PRES-707667.

B. Glass Scintillator Host Materials

1. N. Adelstein and V. Lordi, "Understanding Conductivity in Glasses via First-Principles Study of Localized States," poster OO3.26 presented at *Materials Research Society Fall Meeting*, Boston, December 4, 2013; LLNL-POST-647198.

2. N. Adelstein, C. Olson, and V. Lordi, “Control of electronic traps in sodium silicate glasses via first-principles study of localized states,” UU10.07, presented at *Materials Research Society Fall Meeting*, San Francisco, CA, December 4, 2014; LLNL-POST-665117.

3. N. Adelstein and V. Lordi, “Correlation of Local Structure and Electronic Properties of Glass Materials,” presented at *American Physical Society March Meeting*, San Antonio, TX, March 2–6, 2015; LLNL-PRES-667826.

4. N. Adelstein, C. Olson, and V. Lordi, “Control of electronic traps in sodium silicate glasses via first-principles study of localized states,” poster presented at *SCINT 2015*, Berkeley, CA, June 7–12 (2015); LLNL-POST-665117.

C. Cd(Zn)Te Dislocations

1. V. Lordi, D. Åberg, M. Skarlinksi, and E. Cho, “Atomic and Electronic Structure of Dislocations in CdTe,” H1.10, presented at *Materials Research Society Spring Meeting*, San Francisco, April 22, 2014; LLNL-PRES-653734.

2. V. Lordi, D. Åberg, M. Skarlinski, and E. Cho, “Atomic and Electronic Structure of Dislocations in Cd(Zn)Te,” R02-5, presented at *IEEE NSS/RTSD*, Seattle, November 10, 2014; LLNL-PRES-653734.

3. **(invited)** V. Lordi, “Electronic Structure of Point Defect-Decorated Dislocations in CdTe and Nucleation of Te Precipitates,” R3C-3, presented at *IEEE NSS/RTSD*, San Diego, October 31–November 7, 2015; LLNL-PRES-679042.

4. K.E. Kweon and V. Lordi, “Point-defect Interaction with Dislocations in CdTe and Possible Mechanism for Nucleation of Te Precipitates,” Paper 7.7, presented at *The 2015 US Workshop on the Physics and Chemistry of II-VI Materials*, Chicago, October 5–8, 2015; LLNL-PRES-677719.

5. **(invited)** K.E. Kweon and V. Lordi, “Interaction of Point Defects with Dislocations in CdTe and Nucleation of Te Precipitates,” poster presented at *Dislocations-2016*, Purdue University, Lafayette, IL, September 19–23, 2016; LLNL-POST-702877.

6. K.E. Kweon and V. Lordi, “Interaction of Point Defects with Dislocations in CdTe and Nucleation of Te Precipitates,” R16-3, presented at *NSS/RTSD 2016*, Strasbourg, France, October 29–November 5, 2016; LLNL-PRES-707163.

ACKNOWLEDGMENTS

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[1] K. Hitomi, T. Onodera, T. Shoji, Y. Hiratate, and Z. He, “TlBr gamma-ray spectrometers using the depth sensitive single polarity charge sensing technique,” IEEE Transactions on Nuclear Science **55**, 1781–1784 (2008).

[2] A. V. Churilov, G. Ciampi, H. Kim, L. J.. Cirignano, WM. Higgins, F. Olschner, and KS. Shah, “Thallium bromide nuclear radiation detector development,” IEEE Transactions on Nuclear Science **56**, 1875–1881 (2009).

[3] H. Kim, L. Cirignano, A. Churilov, G. Ciampi, W. Higgins, F. Olschner, and K. Shah, “Developing larger TlBr detectors-detector performance,” IEEE Transactions on Nuclear Science **56**, 819–823 (2009).

[4] I. B. Oliveira, F. E. Costa, P. K. Kiyohara, and M. M. Hamada, “Influence of crystalline surface quality on TlBr radiation detector performance,” IEEE Transactions on Nuclear Science **52**, 2058–2062 (2005).

[5] K. Hitomi, Y. Kikuchi, T. Shoji, and K. Ishii, “Polarization phenomena in TlBr detectors,” IEEE Transactions on Nuclear Science **56**, 1859–1862 (2009).

[6] A. M. Conway, L. F. Voss, A. J. Nelson, P. R. Beck, T. A. Laurence, R. T. Graff, R. J. Nikolic, S. A. Payne, H. Kim, L. J. Cirignano, and K. Shah, “Fabrication methodology of enhanced stability room temperature TlBr gamma detectors,” IEEE Transactions on Nuclear Science **60**, 1231–1236 (2013).

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