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Correlation between Local chemistry, Bottleneck size, and Lithium conductivity in perovskite solid electrolytes

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Solid-state lithium batteries based on inorganic solid electrolytes have gained increasing attention, attributed to their enhanced safety and excellent energy density [1]. Various structural features, such as composition, structural order, or various defects, directly impact the overall ionic conductivity. [2] As an example, the degree of La/Li ordering and domain/grain boundary in lithium-lanthanum titanate Li3xLa2/3-xTiO3 (LLTO) significantly affect the ion conductivity [3,4]. Because oxygen (O) bottlenecks, which are formed between four neighboring TiO6 octahedra, serve as pathways for Li+-ion migration [5], studying local structural features that affect this bottleneck size becomes essential for obtaining descriptors for high ionic transport and designing structures with high performance.
In this presentation, we will show the local structural characteristics of LLTO and highlight the connection between local environments and Li+-ion mobility, using a combination of aberration-corrected scanning transmission electron microscopy (STEM), multislice ptychography, DFT/MD calculations. First, the simultaneously obtained annular dark field (ADF) and integrated differential phase contrast (iDPC) images reveal a reduction in bottleneck size with the increased La(/Li) occupancy. Second, multislice ptychography reconstructions enable the direct observation of O displacements coupled to the neighboring A-site occupancy. Third, investigation through DFT/MD, we will show that the Coulombic forces applied from neighboring cation chemistry towards the bottleneck determine O displacements and O bottleneck size, which is found to be correlated between bottleneck size and Li+-ion migration behavior. These results help establish a robust understanding of the linkage between local chemistry, structure, and ionic conductivity.

Improvement of CdTe Solar Cells Using Patterned Al2O3 Reflectors

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CdTe solar cells have emerged as a leading photovoltaic (PV) technology in the commercial market today due to their excellent optical absorption, operational reliability, and fast manufacturing processes. Recent advancements in front-contact optimization have yielded impressive results, with a short-circuit current (Jsc) of 31.7 mA/cm2 and a fill factor (FF) of 78.5 %, approaching their theoretical maximum values. However, the open-circuit voltage (Voc) remains within the range of 0.8 V to 0.9 V, significantly below the theoretical limit of approximately 1.2 V.
This study investigates innovative back-contact architectures utilizing patterned Al2O3 reflectors. We explore how the configuration of microholes on Al2O3 can enhance the collection of majority carriers through point contacts (metal/CdTe) while preserving surface passivation (Al2O3/CdTe). We apply the same geometry to as-grown and post-annealed CdS/CdTe solar cells to examine the interaction between back-contacts and the CdTe absorber materials. The post-annealed CdTe samples, derived from the as-grown sample set, undergo additional CdCl2-activation processes, effectively passivating various defects (e.g., point defects, dislocations, 2D structural defects), resulting in an improved quality of the CdTe absorber. Our analysis reveals that in as-grown CdTe devices, losses in fill factor (FF) and short-circuit current (Jsc) are primarily associated with the extent of Al2O3 coverage (Al2O3/CdTe). In contrast, post-annealed devices notably enhance these parameters when the microhole point-contact area exceeds 10 %. We employ cathodoluminescence analysis to confirm increased radiative recombination with Al2O3. Additionally, we analyze the Voc trend with the contact fraction (Au/CdTe) of the patterns. Our results suggest a delicate balance between the impact of Al2O3 reflectors on passivation and selectivity and the inherent properties of the CdTe absorber influencing lateral transport.

Thermal Conductivity of High Al Content AlGaN Multiple Quantum Well Heterostructures

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High-Al content AlxGa1-xN heterostructures provide a platform for UV-light emitting diodes (LEDs) and laser diodes (LDs) well into the UV-C regime (200 – 280 nm). However, multiple quantum-well (MQW) structures commonly employed in LEDs and LDs exacerbate self-heating, owing to the multiple interfaces and boundaries which significantly scatter phonons, limiting thermal conduction through these materials [1, 2]. Addressing thermal management will become more critical as the output power of UV emitters increases. In this paper, we discuss the impact of AlGaN-based heterostructure design on thermal conduction.
The effective thermal conduction (κeff) of six AlGaN MQW structures grown by metalorganic chemical vapor deposition (MOCVD) on bulk AlN substrates was measured by Time-domain Thermoreflectance (TDTR). Samples A-C in Set 1 consisted of 11-period MQWs of 2 nm Al0.55Ga0.45N wells with 6 nm Al0.85Ga0.15N barriers (A), 3 nm AlN barriers (B), or 6 nm AlN barriers (C). Samples D-F in Set 2 had 8 periods of 0.6 nm Al0.61Ga0.39N wells (D), 8-periods of 1.35 nm Al0.61Ga0.39N wells (E), and 6-periods of 2 nm Al0.61Ga0.39N wells (F), all with 7 nm AlN barriers. When the number of periods is the same (Set 1), the κeff is most sensitive to the percentage of the structure composed of AlN, with κeff of Sample A (3 ± 0.5 W/mK) < B (4.5 ± 0.6 W/mK) < C (5.4 ± 0.6 W/mK). However, for structures with similar AlN barrier and well thickness, comparison with Set 2 implies that the number of periods has the most significant effect on κeff. Both sample E and F in Set 2 possess a value of κeff higher than all the samples in Set 1. The κeff of Sample F was 8 ± 1 W/mK, which is comparable to the thermal conductivity of thin (< 200 nm) high-Al content