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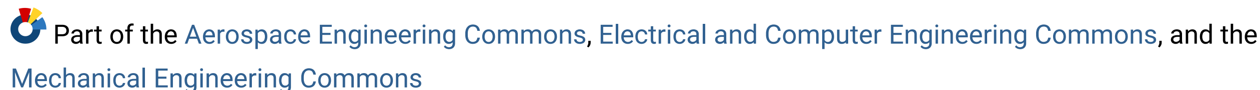
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E. Olugbade et al., "Oxidation Layer Formation on Aluminum Substrates with Surface Defects using Molecular Dynamics Simulation," *2023 IEEE Symposium on Electromagnetic Compatibility and Signal/Power Integrity, EMC+SIPI 2023*, pp. 88 - 93, Institute of Electrical and Electronics Engineers, Jan 2023.
The definitive version is available at https://doi.org/10.1109/EMCSIPI50001.2023.10241439

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Oxidation Layer Formation on Aluminum Substrates with Surface Defects using Molecular Dynamics Simulation

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2023 IEEE Symposium on Electromagnetic Compatibility & Signal/Power Integrity (EMC+SIPI) | 979-8-3503-0976-8/23/$31.00 ©2023 IEEE | DOI: 10.1109/EMCSIPI50001.2023.10241439

***Abstract*—Aluminum oxide layer affects the integrity of electrical contact and can contribute adversely to passive intermodulation (PIM) behavior in radio frequency (RF) devices, necessitating a need for understanding its formation mechanism and realistic estimation of its thickness. Using ReaxFF molecular dynamics simulation technique, this study investigated the impact of surface defects on aluminum oxide layer formation. Results reveal that crystallographic orientation did not affect the kinetics of oxidation process of aluminum. However, the reaction kinetics increased significantly with surface inhomogeneities such as cracks, scratches, and grain boundaries. A non-uniform oxide layer with thickness variation in the range of 72-77% was observed due to surface imperfections. Concurrent crack healing and oxidation was observed, where the crack tips acted as sites for oxygen diffusion, thus increasing oxidation kinetics. The observations from this simulation agree with experimental reports and have important implications for optimizing the contact integrity in RF devices and for PIM control.**

***Index Terms*—Aluminum oxide layer, surface defects, molecular dynamics simulation, electrical contact integrity, PIM**

I. Introduction

Aluminum is a highly desirable material in RF components due to its superior electrical conductivity and mechanical properties. However, exposure to air leads to the formation of an oxide layer on the surface, which can greatly impact the performance of RF devices. One of the most significant effects of the oxide layer is the alteration of electrical conductivity at the metal-to-metal interface, resulting in contact non-linearity and passive intermodulation (PIM). PIM is a critical issue in RF devices as it can significantly impair their performance. Studies have demonstrated that even minor variations in oxide layer thickness, L as small as 1 nm, can result in a substantial decrease in zero-bias conductance, G by as much as three orders of magnitude (Fig. 1) [1]. This can be attributed to the oxide layer's electrically insulating properties and the fact that conductance is heavily dependent on quantum tunneling [2], making it critically dependent on oxide layer thickness. A variety of experimental methods, including scanning electron microscopy (SEM), x-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM) have been employed to study the growth of oxide on aluminum surfaces, and to characterize the resulting oxide layers [3] [4] [5] [6] [7]. Meanwhile, the thickness of air-formed aluminum oxide layer has been reported to range widely in the literature, typically between 2 to 4 nm, [8] [9] [10], yet there is still much that is not understood about how the oxidation mechanism is affected by defects on the aluminum surface. In recent years, molecular dynamics (MD) simulations have been increasingly used to study the formation of aluminum oxide to gain a deeper understanding of the underlying mechanisms. Several studies [11] [12] [13] [14] have used MD simulations to examine the oxidation process of aluminum nanoparticles, identifying different stages of the process such as initial oxygen diffusion, accelerated oxygen uptake due to localized melting of alumina, and direct oxidation through aluminum atom ejection into surrounding oxygen atoms. Despite the valuable insights gained from previous studies, it should be noted that the impact of defects such as cracks, scratches, or grain boundaries in surface structure of aluminum was not considered, which is unrealistic. To gain a more comprehensive understanding and make more accurate predictions about the behavior of aluminum oxidation under different conditions, this study investigates how surface inhomogeneities and defects contribute to variation in oxide growth thickness and identifies the variations in oxide formation mechanism caused by defects. The results presented in this study have important implications for understanding the characteristics of aluminum oxide layer in electrical contacts in RF devices for the control of PIM.

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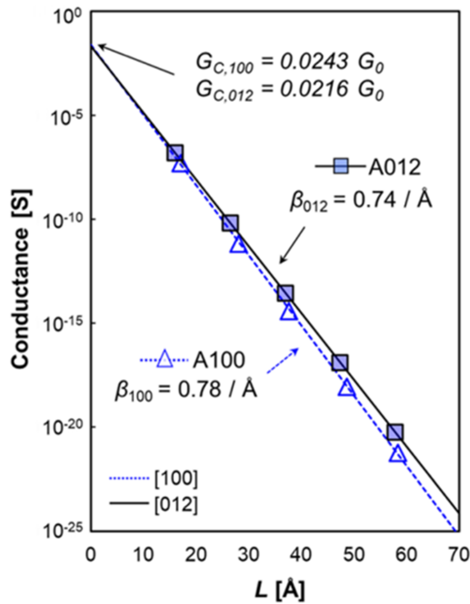

Fig. 1. Thickness dependence of the conductance calculated for Platinum electrode of facets (100) (solid line with filled squares) and (012) (dotted line with hollow triangles) under zero bias limit, where β_{100} and β_{012} are tunneling decay rates, and G_C and G_0 are effective contact conductance and nominal conductance without oxide layer respectively. [1]

II. METHODS

A. Computational method

The open-source LAMMPS code [15] linked with ReaxFF [16] was used to run all simulations including the oxidation of aluminum and foreign components. The ReaxFF has been designed for a variety of chemical systems. In the current investigation, the framework with ReaxFF settings created by Hong et al. [12] was used. More recent works by other groups [17] [18] [19] [20] demonstrated that such a framework offered a method for understanding the thermal oxidation of aluminum by accurately describing the interaction between the metal and oxygen gas. The simulated density of bulk Al was compared to an experimentally known value with an error of 0.06%, essentially agreeing with the experimental result, as a validation of the ReaxFF reactive forcefield for use in this work. The ReaxFF reactive force field is based on the bond order/distance relationship proposed by Tersoff [21]. The ReaxFF force field is generated from a quantum mechanics-based parametrization [22] and is updated every iteration to include covalent bonds, valence bonds, and torsion angles. To ensure that chemical reactions are accurately represented in ReaxFF-MD simulations, it is necessary to use a timestep that is lower than the highest frequency of the molecules being simulated. This is typically on the order of 0.5-1.0 fs and allows the simulation to smoothly capture the dynamics of the reactions as they occur [23]. All our simulations used a 0.5fs timestep, and the adsorption, dissociation, and diffusion of oxygen molecules were accurately modeled.

B. Model configurations

a) Model with no defect: The accuracy of an oxidation simulation is being validated using two types of face centered cubic (FCC) aluminum crystals oriented in (100) and (111) planes as a reference (Fig. 2a, b). Importantly, these crystals are free from defects, indicating their structural perfection. The use of these crystals also allows for the validation of the accuracy of the oxidation simulation using the ReaxFF reactive forcefield method.

b) Microcrack and scratch models: During machining operations, the material being processed is subjected to high levels of friction and thermal stresses that can cause cracks and scratches on the surface of the material. A set of Mode I cracks formed by applying shearing stress of 26 GPa and stress intensity factor of 40 MPa.m$^{1/2}$ were modelled on the aluminum sample resulting in a crack length of 3 nm (Fig. 2e), an average crack size commonly observed in aluminum samples [24]. To maintain the integrity of the cracks during the equilibration phase, the atoms adjacent to the cracks were frozen. As for the model with surface scratch, a few atoms were removed from the surface of an Al crystal up to a depth of 3nm as seen in Fig. 2c. To study the impact of crack depth on oxide formation, we created an additional model with a crack depth of 20 nm. This model was later used to explain the process of crack healing found during the oxidation process.

c) Grain boundary model: Grain boundaries can have significant impact on the behavior of the material dynamics in oxidation reactions at the locations where they are found [25]. In our work, we sought to investigate the influence of grain boundaries on the oxidation reaction of aluminum. To do this, we modeled a polycrystalline structure obtained from Voronoi tessellation protocol. The crystals were given a random orientation and as a result, they form diverse grain boundaries at the surface of a flat Al substrate (Fig. 2d). The grain boundary model has a dimension of 10nm×10nm×3nm with 181,132 atoms.

C. Simulation setup

In this study, we utilized the Atomsk software [26] to create models with defects on aluminum. A vacuum was created on top of the aluminum in the z-direction to represent the surface of the aluminum. Then, these models were relaxed in an isothermal-isobaric (NPT) ensemble and a canonical (NVT)) ensemble at 300 K in preparation for oxidation simulations. For the oxidation simulation, oxygen molecules were introduced into the vacuum region near the surface of the aluminum. The starting point for these oxygen molecules was randomly chosen within a designated region within the vacuum. As the oxygen molecules approached the surface of the aluminum, they were allowed to dissociate before another oxygen molecule was released into the simulation box to maintain a smooth dynamic of the system and to prevent collisions between oxygen molecules, which could increase the kinetic energy and temperature of the system. Oxidation run was performed over 4,000,000 timesteps at which the oxidation process in all the models had reached a limiting

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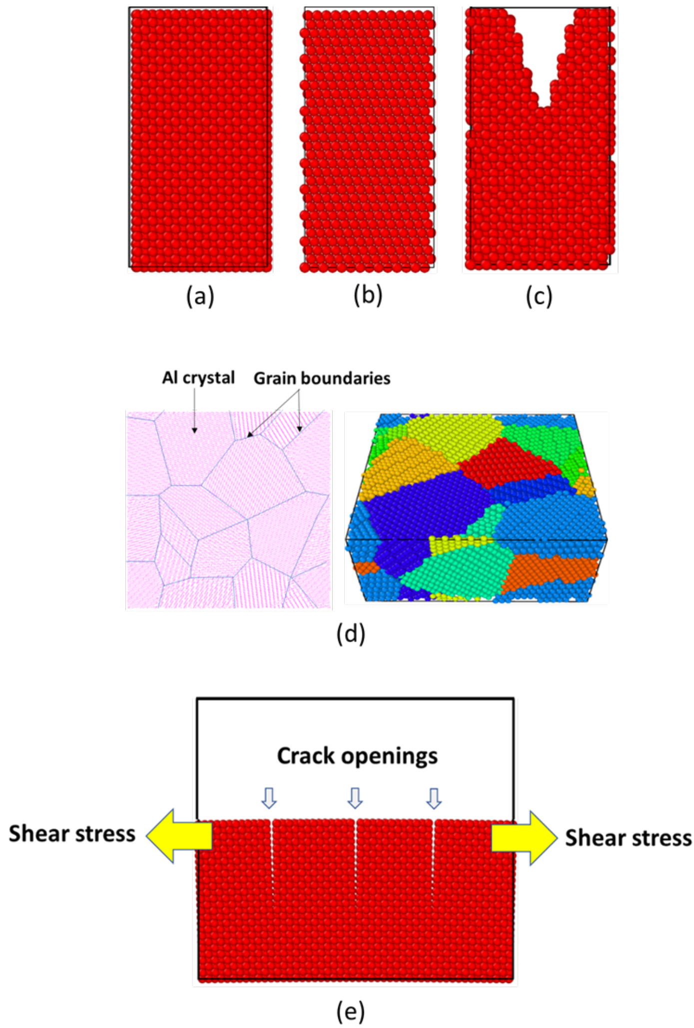

Fig. 2. Models for oxidation simulation. (a) Al(1 0 0) crystal with no defects, (b) Al(1 1 1) crystal with no defects, (c) model with surface scratch, (d) grain boundary model and (d) microcrack model

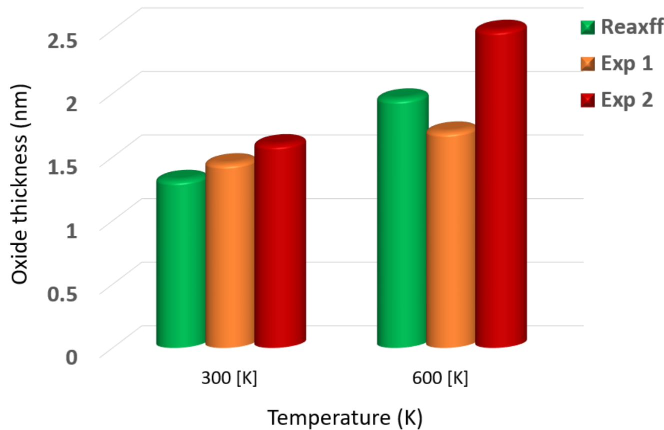

Fig. 3. Comparison of the growth of the oxide film with temperature increase in the ReaxFF and experiment

point. The limiting point of the oxidation rate may provide some insight into the time frame over which the oxidation process occurs and the rate at which it occurs. Periodic boundary conditions were applied along the x and y axes of the simulation box, while the z-direction was fixed.

III. Results and Discussion

A. Validation of ReaxFF Force Field for Oxidation of Aluminum

For validation of the ReaxFF for the study of Al oxidation mechanism, experimental measurement [27] of oxide layer thickness with an impact of temperature increase was utilized. Fig. 3 presents a comparison of the growth of the oxide film as a function of temperature increase in both computational (ReaxFF) and experimental approaches. It is apparent that the oxide thickness increases continuously with increasing temperature, as observed in the experimental data [26] [29] [30]. Overall, these results suggest that the ReaxFF method can accurately capture the key features of the oxidation process for aluminum materials with respect to temperature. Also, the simulated density of bulk Al compares to an experimentally known value with an error of 0.06%, essentially agreeing with the experimental result.

B. Kinetics of oxide film growth

As shown in Fig. 4, the intake of oxygen increases more rapidly but as the formation of the oxide layer tends to its limiting value, the influx of oxygen into the film is impeded. From our simulation results, we observed that the potential energy of the system decreased significantly as the oxygen was consumed, indicating that the oxidation process is exothermic. This exothermic reaction leads to the formation of hot spots on the surface of the aluminum substrate. However, the thermostat settings in the system function as a thermal bath, quickly transferring and regulating the heat energy generated. The temperature in the system is regulated by the thermostat and does not significantly increase just as the case observed experimentally, due to the heat being transferred and dispersed to the surroundings through convection and conduction [14] [31]. The formation of void spaces facilitates the movement of oxygen into the sublayer atoms of aluminum and accelerates the oxidation process by lowering the energy barrier for oxygen diffusion.

C. Effect of crystallographic direction

The results shown in Fig. 4 indicate that the thickness of the oxide layer that forms on the surface of aluminum is similar, regardless of whether the aluminum has a (100) or (111) crystallographic orientation. From the figure, we see that the thickness tends to a limiting value of 1.3 nm in both models at 300 K. This suggests that the mechanism by which the oxide layer grows is not affected by the crystallographic orientation of the aluminum surface. This finding is consistent with previous experimental research and simulations [28] [32] [33] [34]. Based on these results, it can be inferred that crystallographic orientation does not significantly influence the

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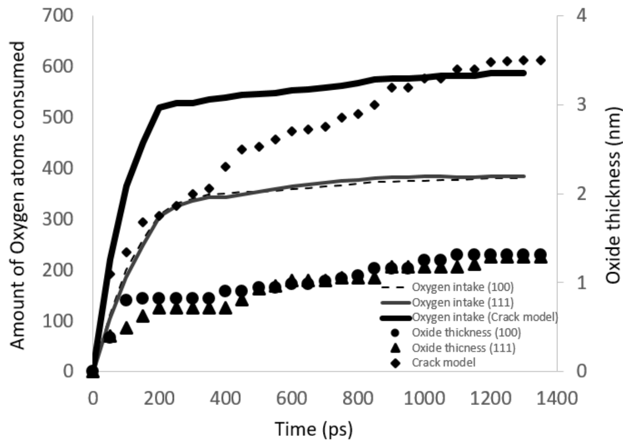

Fig. 4. Oxidation kinetic curves showing amount of Oxygen atoms consumed with time for the two crystallographic planes and the crack model (plotted with lines), and the evolution of oxide layer thickness (plotted with dots) in Al(1 0 0) and Al(1 1 1) crystallographic planes.

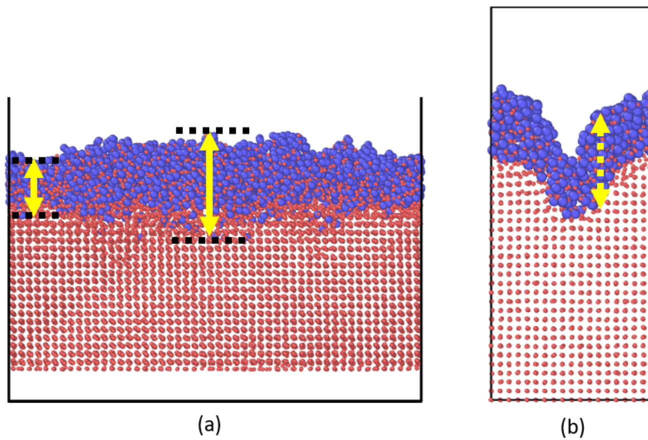

Fig. 5. Snapshot of oxide layer formed on (a) crack model and (b) scratch model after oxidation formation has reached a limiting thickness

variation of the oxidation layer. Therefore, for the purpose of studying the impact of defects on the oxide layer growth in subsequent models, only one crystallographic direction will be utilized.

D. *Impact of surface cracks and scratch on oxide thickness*

Our results showed that the presence of surface imperfections and inhomogeneity significantly impacted the thickness of the oxide layer and the morphology of the oxide layer formed on the aluminum substrate. We observed a non-uniform oxide layer thickness in the presence of surface cracks, with a maximum oxide thickness that was 77% larger than in the absence of cracks, being as thick as 3.5 nm to 4 nm in models with cracks and scratch respectively (Fig. 5). The increased oxide thickness observed can be explained by considering that surface imperfections create additional sites and larger surface area in aluminum substrate for increased oxygen interaction, resulting in favorable kinetics for the

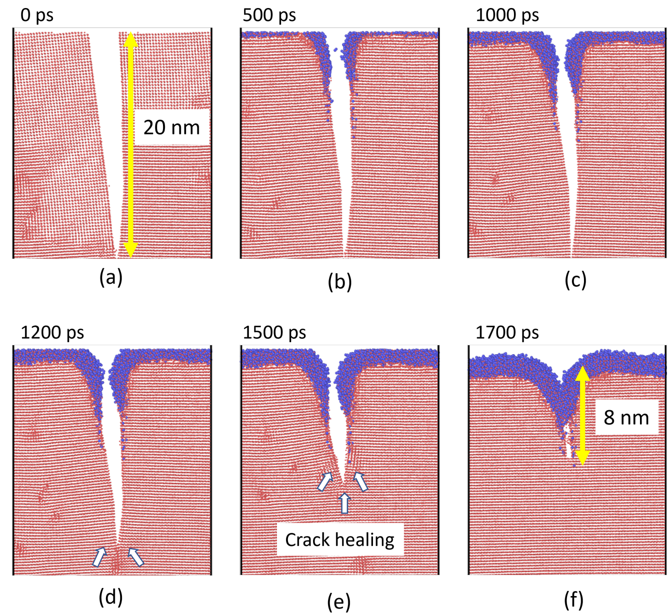

Fig. 6. Snapshots of the evolution of oxidation process in Aluminum with 20-nm crack depth. Oxidation and crack healing are seen to occur concurrently.

oxidation reaction. The study also delved into the process of healing of the surface cracks at the onset of the oxidation process. We observed in the model with crack that, during the oxidation process, the surface cracks began to heal as the openings gradually closed due to atomic relaxation at the crack tip. Fig. 6 (d) and (e) clearly show the occurrence of crack healing. This healing phenomenon is consistent with previous experimental reports in the literature [35] [36]. However, the rate at which they closed was not fast enough to keep pace with the initial oxidation rate. Consequently, the crack openings remained as sites for oxygen diffusion, thereby allowing for a continuous penetration of oxygen atoms. Also, from Fig. 6, which had an initial crack depth of 20 nm, an oxide layer depth of about 8 nm is estimated around the crack region. So, the more severe the crack on the metal surface, the deeper the oxide layer can get. An interesting observation from the scratch model is the formation of severe, rough morphology of the surface. It appears that there was no healing of the defect as in the case of surface crack. To evaluate the kinetics of the oxidation process, we compared the rate of oxygen consumption in the model with surface scratch and that of perfect crystal. The results showed that the rate of oxidation was significantly faster in the former than in the perfect crystal model. As seen in Fig. 4, the crack model consumed more oxygen than the perfect crystalline model, and the consumption of oxygen happened much faster. One possible explanation for this observation is that the presence of scratch creates additional sites and larger surface area for oxygen interaction with the aluminum atoms, facilitating the oxidation reaction.

Furthermore, we characterized the structures of the sim-

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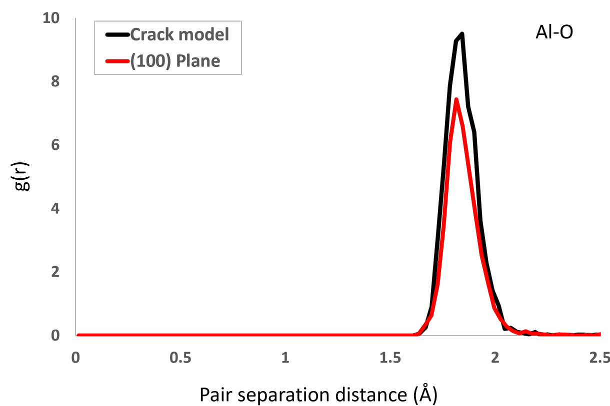

Fig. 7. Radial distribution function of aluminum oxide layer.

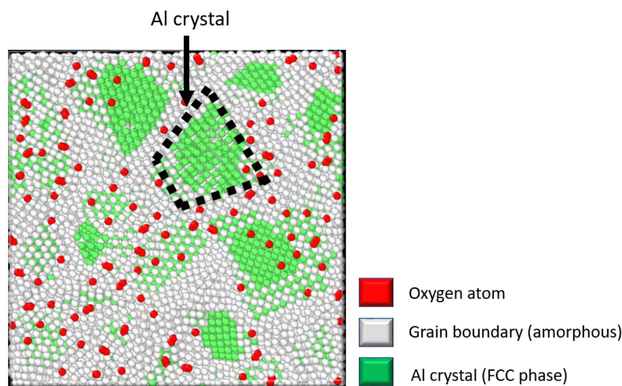

Fig. 8. Snapshot of oxygen migration in the grain-boundary model. Coloring is based on common neighbor analysis of existing crystalline environment.

ulated oxide layer of the model with surface imperfection (scratch) and the perfect crystal in terms of radial distribution functions (RDF) (Fig. 7). The results of the RDF analysis revealed that there was no significant structural variation in the oxide layers attributable to the presence of surface imperfections. Specifically, the Al-O bond distance, which is a measure of the distance between aluminum atoms and oxygen atoms in the oxide layer, was about 1.8 Å in both the perfect crystal and crack models. This value agrees with experimental measurements obtained from diffraction methods [37] [38] and confirms an amorphous structure of the oxide layer formed in both cases. This indicates that while surface imperfections would contribute to increase in oxide layer thickness, it does not seem to cause significant structural variation in the oxide layer.

E. Effect of grain boundaries

We utilized a polycrystalline aluminum (Al) substrate as a model system. Through the visualization of oxygen migration on the surface of the metal (Fig. 8), it has been observed that there is a higher population of oxygen migration at the grain boundaries, as opposed to the perfect crystalline regions. This observation is consistent with previous experimental studies [36] [39] and suggests that grain boundaries provide a favorable site for oxidation progression to occur. It is theorized that this phenomenon is driven by the migration of atoms at the grain boundaries, as well as the diffusion of oxygen atoms through the grain boundary [40] [41]. As a result of this increased oxidation activity at the grain boundaries, it has been found that the oxide layers formed at these locations are thicker in size than those found within the bulk grains. In some cases, a maximum increase of 72% in oxide layer thickness was observed.

IV. Conclusions

In this study, the effects of defects on the variation of the oxide layer in aluminum crystals were investigated. The impact of crystallographic orientations on aluminum oxidation was examined and it was found that the thickness of the oxide layer is approximately the same regardless of the crystal orientation of aluminum, and is limited to about 1.3 nm at 300 K. Also, the study discovered that the presence of surface defects has significant impact on the thickness of the oxide layer and the kinetics of the oxidation process. Non-uniform oxide layer thickness and a faster oxidation rate were observed in the presence of surface defects. It was also noted that surface cracks began to heal during the oxidation process but at a slower rate than the initial oxidation rate and the crack openings remained as sites for oxygen diffusion. Additionally, the relationship between grain boundaries and aluminum oxidation was studied and it was observed that oxygen migrated and accumulated at the grain boundaries rather than at the surface of the fully crystalline regions. The observations from this study have important implications for optimizing contact integrity in RF devices and for improving the understanding of PIM characterization and analysis.

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