Supporting Information

Liquid-phase exfoliated SnS as a semiconductor coating filler to enhance corrosion protection performance

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Supporting Information



Figure S1. Fabrication process of copper substrate with PVB/SnS composites.

Simulation methodology

Molecular simulations (MD) have been performed using commercially available software, Material Studio 8.0, purchased from Accelrys Inc.[1] The structure of PVB chain and molecules of SnS were generated and optimized through the Forcite module. The energy minimized structures of PVB (5 chains) and SnS (in different wt%) were used for the construction of different composites through Amorphous Cell Tools of Material Studio. The optimization procedure follows convergence criteria: 2.0×10^{-5} kcal/mol for energy, 0.001 kcal/mol/Å for force, and 1.0×10^{-5} for displacement. After the geometry optimization, MD calculation with NVT ensemble and Universal force field (UFF) was performed at time step of 1.0 fs up to total 5.0 ns, among which Andersen algorithm themostat with 1.0 Collision ratio was used to maintain the temperature of the system at around 298 K. The flow chart of simulation is shown in Figure S2.



Figure S 2. Flow chart of the simulation method to calculate the properties of PVB/SnS based coatings.

1. Modeling of equilibrated bulk PVB structure

Initial bulk PVB periodic structure is constructed through Amorphous cells Module of Material Studio with 5 chains of PVB. The structure is subjected to energy relaxiation using Forcite module for 1000 iterations. Then, NVT simulations are performed at 298 K at time step of 1.0 fs up to total 5.0 ns, and the lowest potential energy frame is selected as equilibrated bulk PVB structure. The calculated density of the equilibrated structure is consist with the experimental values for PVB reported in previous works, which is 1.1 g/cm³.[2]

2. Generation of composites coating

The equilibrated structure of bulk PVB (5 chains) and SnS (in different wt%) are used for the construction of different amorphous cells. Then the composites perodic structure is subjected to perform the minimization, energy relaxiation, and equilibration in sequence. And the equilibrated PVB/SnS composite is obtained.

3. Simulation of coating-metal interation energy

At first, we exported the FCC (Face Centered Cubic) crystal lattice cell of copper (Cu), which is of lattice parameters: a = b = c = 3.6147 and $\alpha = \beta = \gamma = 90^{\circ}$, from the Material Studio 8.0 database. The exported lattice is then cleaved along the plane of (1 1 1) for Cu[3]. The vaccum thickness of 10 Å is bulid on the surface of lattice. The surface formed is then energy minimized and structure relaxed using Forcite module. Next, we place the PVB/SnS composite coating to the Cu surface through "Build Layer" function of Material Studio. The thickness of 25 Å vaccum is introduced above the composites for eliminating the interaction between periodic PVB/SnS-Cu systems. Also, the geometry is optimized within the convergence criteria of 2.0×10^{-5} kcal/mol for energy, 0.001 kcal/mol/Å for force, and 1.0×10^{-5} for displacement. Finally, NVT dynamics with UFF potential is performed at time step of 1.0 fs up to total 5.0 ns.



Figure S3. The molecular formula of PVB used in this work. For simplification, $X_{80}Y_{18}Z_2$ was applied as simulation model, where X represents Butyryl, Y represents Hydroxyl Content and Z represents Acetate Content.



Figure S4. (Left) Illustration of the PVB/SnS-Cu system consisting of Cu (1 1 1) crystal as the first layer (shown in brown mini-spheres) and PVB/SnS_x (x=0, 0.05, 0.1, 0.2, 0.5, and 1) at time t = 0 ps and (Right) Final two layered structure post-MD run of 500 ps.

Reference for supporting information

 [1] b.D.S.B. Material Studio^{TM,} UK (Accelrys[®]) in, pp. <u>http://accelrys.com/products/materials-studio/</u>,.
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