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Quantum mechanical modeling of hydrogen assisted cracking in aluminum QING PENG, Rensslaer Polytechnic Institute, YI SUN, GANG LU, California State University Northridge — We report multiscale quantum mechanical modeling of hydrogen assisted cracking in aluminum which is central to H embrittlement phenomena. We find that dislocation emission and brittle cleavage can occur simultaneously. H embrittlement takes place when H occupies the top sites on the crack front surface and even a very low H coverage at 0.2 monolayers can lead to brittle cleavage. H atoms adsorbed on the crack surfaces tend to suppress dislocation emission, whereas the solute H atoms on the slip plane can promote dislocation emission. Top-site H atoms at the front surface are found to facilitate the migration of other H atoms towards the front surface, providing a mechanism for H accumulation at the crack tip. The study resolves a long-standing puzzle of why H embrittlement could occur in Al where the equilibrium H solubility is extremely low under normal conditions.

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