Electron Scattering Studies of atomic Mo and MoS_2

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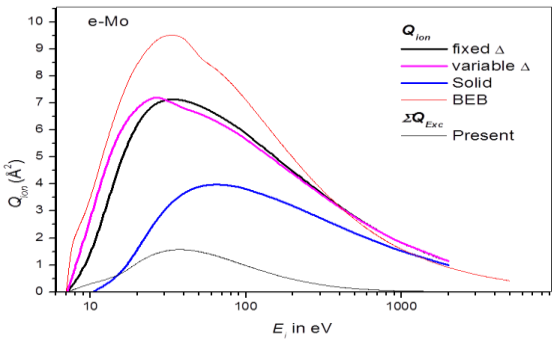
Synopsis This paper reports initial theoretical findings of electron scattering by two plasma important targets: 1) atomic molybdenum and 2) Molybdenum Sulfide MoS_2. Spherical Complex potential formalism is used to derive total as well as inelastic cross-sections. The CSP-*ic* method, developed by us, is employed to extract ionization cross section from the inelastic cross section. A variant of the method is also considered.

The plasma equipment for plasma etching, deposition and cleaning typically use partially ionized, low pressure plasmas to provide activation energy to dissociate and ionize feedstock gases. The resulting radicals and ions interact with the semiconductor surface, either removing or adding material, to define the desired features or modify the surface. This requires the modeling efforts to simulation for these processes. Essential input for modeling these processes in plasma physics consists of complete cross section data for all elastic and inelastic interactions. In fusion plasmas many kinds of impurity ions exist due to the sputtering of the wall materials. The understanding of the atomic processes of the elements with industrial importance such as Mo is also essential to control the impurity ions in plasmas.[1]

The calculations on atomic Molybdenum ~~is~~ are also of interest in divertor studies in several experimental facilities, where a spectroscopic determination of impurity influx from the molybdenum surface is needed. One of the outstanding challenges in applied plasma physics is the development of non-mercury gas discharges for lighting. The discovery of graphene nearly a decade ago has stimulated intensive research efforts in atomically thin, two-dimensional (2D) crystals, such as transition-metal dichalcogenide (TMD) semiconductors and boron-nitride (BN).Recent experimental and theoretical work shows that these layered TMDs undergo a transition from indirect to direct band-gap when their thickness is reduced from bulk to monolayer, leading to a pronounced photoluminescence (PL). Among this family, molybdenum disulfide (MoS_2) is one of the most stable layered TMDs [2]. Atomically thin molybdenum disulfide (MoS_2) offers potential for advanced devices and an alternative to graphene due to its unique electronic and optical properties [3].

In this context, the present paper reports theoretical findings on electron scattering with free atomic molybdenum as well as MoS_2 in solid. Presently we determine total ionization cross section Q_{ion}. We have employed the well-known spherical complex (optical) potential formalism i. e. (SCOP), which provides total elastic cross section Q_{el} and its inelastic counterpart Q_{inel} which includes Q_{ion}. We have already developed a method to extract ionization cross sections Q_{ion} from calculated inelastic cross sections Q_{inel}, by introducing a ratio function as in [4]. The calculated cross sections are examined as functions of incident electron energy along with available comparisons. In general there is a decrease in the Q_{ion} in going from the gas to the solid phase of a target. Detailed analysis of the results will be presented in the Conference.



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