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Cage motion of Iron (Fe) in Silicon (Si)

Due to its negative impact on semiconductor devices, iron (Fe) is one of the most thoroughly investigated impurities in silicon. It is a usual unintended impurity in silicon manufacturing, functioning as a fast diffuser and severely lowering carrier lifetimes, especially harmful for solar cells applications [1]. It is still unclear how defects or other impurities interact with substitutional and interstitial Fe under implantation conditions. Obtaining an understanding of the behaviour of metal impurities, such as Fe, in silicon can result in methods for improving gettering procedures, which transfer metallic impurities to less hazardous areas of devices. This motivates investigation of the fundamental properties and behaviour of Fe in silicon at the atomic scale. Techniques such as emission Mössbauer spectroscopy and emission channelling provide valuable insights into the behaviour of dilute probe atoms in these contexts. We demonstrate, using 57Fe Mössbauer spectroscopy following implantation of 57Mn ($T_{1/2}$ = 1.5) min. that substitutional Fe in silicon is not located on the ideal substitutional site, but exhibits cage motion or jumps via saddle sites, located 0.17(3) Å from the ideal substitutional site. In the temperature range from 300 K to 500 K, the jump rates follow an Arrhenius behaviour, with rates in the vicinity of 10^7-10^8 Hz and an activation energy of 0.18(3) eV. Our data also suggest compressive strain on substitutional sites and relaxing strain on interstitial sites when the implantation is below ~450 K. These findings provide new insights into the atomic-scale behaviour of Fe in silicon, which is essential for improving material processing and device performance.

Notes

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