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Impurity Segregation at the Si/SiO_2 Interface A. G. MARINOPOULOS, K. VAN BENTHEM, S. RASHKEEV, S. J. PENNYCOOK, S. T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235 and Oak Ridge National Laboratory, Oak Ridge, TN 37831 — It is a widely known fact that impurities tend to segregate at interfaces between two materials. Here we report first-principles density-functional calculations and Z-contrast scanning transmission electron microscopy and demonstrate that impurities may either segregate or avoid the Si-SiO_2 interface, depending on their chemical identity and which side of the interface they originate from. Segregation mechanisms can be very different depending on the chemical nature of the impurity. In particular, we show that in the "alternate dielectric" Si-SiO_2-HfO_2 structure, which is highly promising for cutting-edge Si-based metal-oxide-semiconductor FET, individual Hf atoms, which enter the SiO_2 interlayer during high-temperature annealing, avoid the interface: both Z-contrast imaging and theory find that individual Hf atoms stay away from the nominal interface by about 2.5 to 3 Å. In contrast, theory finds that Hf as a substitutional impurity in Si can reach the interface and in fact segregates in a single plane at substitutional sites at the nominal interface plane. This behavior is in contradiction to other dopant impurities such as As or P, which segregate at the interface only in the form of substitutional dimers in which the impurities achieve threefold coordination. (AFOSR/DOE in part)

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