Growing precisely aligned epitaxial nanodots and other nanostructures

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Matching integral multiples of lattice planes provides a new paradigm for epitaxy across the ‘misfit’ scale that promises to increase the scope of materials for smart devices.

Next-generation nanotechnology depends on our ability to integrate functional structures (ranging from nanodots to nanolayers) on a computer chip. Such devices will allow sensing, manipulation, and response (smart) operations more efficiently than their current, hard-wired counterparts. But progress in this area is contingent on successful fabrication of thin-film heterostructures of dissimilar materials with varying lattice misfits. Small lattice misfits (< 7%) could be handled by existing concepts of lattice-matching epitaxy (thin-film growth). However, larger lattice misfits urgently require new thinking. In addition, a host of other devices, such as LEDs based on gallium indium nitride/gallium nitride/sapphire heterostructures, involve large lattice misfits (> 15%).

Here, we introduce a novel paradigm for handling epitaxial growth across the misfit scale.\(^1\)\(^-\)\(^3\) In domain-matching epitaxy (DME), we consider the matching of lattice planes between the film (planar spacing \(d_f\)) and the substrate (spacing \(d_s\)), which could vary for different directions of the film-substrate interface. The misfit is accommodated by matching integral multiples of lattice planes—for example, four lattice planes of the film matching with three of the substrate—and there is one extra half-plane (dislocation) that corresponds to each domain. The misfit can range from very small to very large. This matching of integral multiples of lattice planes may leave a residual strain of \(\varepsilon_r\) given by \(\varepsilon_r = (md_f / n d_s - 1)\), where \(m\) and \(n\) are simple integers. In the case of perfect matching, \(md_f = nd_s\), and the residual strain \(\varepsilon_r\) is zero. If \(\varepsilon_r\) is finite, then two domains may alternate with a certain frequency to provide for perfect matching with no residual strain according to \((m + \alpha)d_f = (n + \alpha)d_s\), where \(\alpha\) is the frequency factor. For example, if \(\alpha = 0.5\), then the \(m/n\) and \((m + 1)/(n + 1)\) domains alternate with an equal frequency. If domain matching is not perfect, epitaxy occurs by accommodating the additional misfit through a change in domain size, controlled by \(\alpha\). In this framework, it is important to realize that the nature of dislocations remains the same. Only their periodicity changes to accommodate the misfit strain. In large misfit systems (>10%), the critical thickness is more than a few monolayers. Consequently, all strain can be relaxed at the outset, and the rest of the film can grow strain-free. We have verified these predictions of DME by detailed high-resolution transmission-electron microscopy (TEM) and in situ synchrotron studies.\(^3\)

Figure 1. Domain-matching epitaxy paradigm. (a) High-resolution transmission-electron-microscope image of a cross-section of titanium nitride/silicon (100): TiN/Si(100). (inset, upper left) Single-crystal diffraction from TiN and Si<110> with a 22% epitaxial interface of misfit. (b) Self-assembled nickel (Ni)/TiN/Si(100) nanostructures. (c) Ni/TiN epitaxial interface with a misfit of 17%.

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Nickel (Ni) and iron platinum (FePt) epitaxial nanodots stand to transform information storage by storing one bit of information in a nanodot. However, these nanodots need to be epitaxial single crystal and precisely oriented to function reliably. We have shown epitaxial growth of Ni nanodots on a silicon 100—i.e., cube plane of silicon—computer chip using nonmagnetic and metallic titanium nitride (TiN) buffer. A misfit of > 22% for cube-on-cube TiN ($a = 0.424\text{nm}$, where $a$ is the lattice constant) epitaxy over silicon ($a = 0.543\text{nm}$) is beyond the critical strain (7–8%) of conventional lattice matching. However, using the DME paradigm, we were able to demonstrate epitaxial growth of TiN on a silicon substrate, as shown in Figure 1(a), where the 3/4 and 4/5 domains alternate in a detailed high-resolution cross-section TEM micrograph. These observations are consistent with our predictions. The micrograph was taken in the $<110>$ zone axis of silicon and TiN. Note the matching of $\{111\}$ extra half-planes in silicon as well as TiN.

Storing information in magnetic nanodots and reading them reliably are major challenges in next-generation storage technology. This challenge requires that nanodots of magnetic materials such as Ni and FePt be grown epitaxially on nonmagnetic substrates. Furthermore, the ability to integrate nanodots epitaxially on Si(100) holds considerable promise for multifunctional devices. Figure 1(b) shows the formation of self-assembled Ni nanodots on a TiN/S(100) substrate. These nanodots are epitaxially aligned with the underlying TiN despite the lattice misfit of > 17% between TiN and Ni ($a = 0.352\text{nm}$); see Figure 1(c). We have also grown epitaxial FePt nanodot structures ordered $\text{L1}_0$ (i.e., face-centered tetragonal) with a $c/a$ ratio of 0.97 (where $c$ is a perpendicular constant). These structures have much higher coercivity ($7.0 \times 10^7\text{ erg/cm}^3$) compared with Ni ($5.0 \times 10^4\text{ erg/cm}^3$). In the case of FePt, the misfit between the nanodots and TiN is ~10%. However, one bit of information can be stored in thermally stable FePt nanodots of size < 5nm at room temperature.

In summary, we have shown that matching integral multiples of lattice planes in DME enables nanostructures across the misfit scale to be grown epitaxially and integrated with Si(100) and other substrates for a variety of functional devices. Further research will focus on the performance reliability of nanostructures and scaleup processing steps.

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**References**