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Article

Direct Visualization of Si and Ge Atoms by Shifting Electron Picoscopy

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Abstract: The picoscopy images of the Si/Ge(100) system were analyzed, and electron cloud densitometry of silicon is presented in this study. The picoscopy is used to distinguish Ge, Si, and other chemical elements because different atoms have different densities of electron clouds. This result is in full accordance with Kucherov's law which states that the current passed through an electron cloud is proportional to the density of the cloud. The picoscopy image has shown Si crystals, Si/Ge solid solution, and their interface as the single crystal without defects. Local deformations in crystals were investigated using methods of direct visualization of individual atoms and measuring the distance of the center of atoms from the node of the crystal lattice. Visual crystallography becomes a new way to study applied functional materials. This is the first publication on the real structure of a silicon atom.

Keywords: Atomograpfy of crystals, Picoscopy, Solid solutions Ge(Si), Electron cloud densitometry, Visual material science, Visual crystallography

1. Introduction

The practical and functional properties of materials are completely determined by the atoms and molecules of which they are composed. Spectroscopy measures the energy properties of atoms and molecules, while X-ray crystallography measures their positions in space. These are indirect (blind) methods. A materials scientist who cannot see atoms is like a builder who cannot see bricks. The picoscopy gives the direct visualization of atoms, molecules, and chemical bonds and shows atoms of silicon [1], diamond [2], graphite [3], and coke [4]. Rudenite, the world's densest substance [5,6] was discovered by imaging atoms with a picoscope. Therefore, to visually recognize atoms of Si from Ge in a solid solution, the picoscopy plays an important technological role.

Superlattices have layered structures that contain an interlayer between different materials. High interest has been paid to the nanostructures of bulk Ge and Si [7], thin Ge films grown on Si(111) [8,9], and Si (100) [10], which is motivated by their high functionality and a broad spectrum of possible applications in electronics and photonics. In particular, field electron emission from bulk Ge and Si [7] or from Ge islands [8] and quantum dots (QD) [9] are considered to be important. However, the study of the functional properties of these materials has a big problem, a lack of visualization of the atoms. However, the picoscopy solves this problem.

2. Experiment

The technology of electron cloud densitometry of atoms and chemical bonds is described in this section. The body of valence electrons cannot be seen with either an optical microscope or a transmission electron microscope. Classical physics does not allow this for two reasons. First, electrons do not have visible bodies. Second, both optical and electron waves exceed the size of an atom. However, quantum mechanics allows us to observe the real shape of the inner and valence electrons. Quantum mechanics shows that the electrons that revolve around the nucleus of an atom have the shape of a cloud which has a density [9]. Kucherov and Lavrovsky [13, 14] invented electron cloud densitometry, the essence of which is that an electron beam, passing through an atom, receives information about the shapes of electron clouds.

Consider two objects of quantum mechanics: (a) an atom with inner and valence electrons and (b) an external electron beam. Quantum mechanical objects have the properties of waves and particles at the same time. When objects are waves, the following equation defines the probability $I(x, y)$ to find the electron at points x, y of the microscope screen [4].

$$J(x, y) = jn\rho(x, y) \tag{1}$$

where $\boldsymbol{j}$ is a plane wave, $\boldsymbol{n}$ is the number of electrons in an electron cloud, and $\boldsymbol{\rho(x, y)}$ the electron cloud density of one electron.

Thus, the plane wave amplitude $\boldsymbol{J(x, y)}$ is proportional to the electron cloud density $\boldsymbol{\rho(x, y)}$ or the thickness of the electron cloud of the atom at the point of the beam passage. The cloud changes the current not by absorption or amplification, but by spatial shift due to the principle of superposition. This is a purely quantum effect, which is absent in electrodynamics. Equation (1) is accurate and not approximated in any way.

Law 1. Thus, the interaction of the electric beam with electron clouds following the principle of quantum mechanical superposition obeys the Kucherov law. That is, the current passed by an electron cloud is proportional to the density of that cloud.

The electron cloud shifts the electron beam. The intensity is not lost but redistributed. When the object under study has the size of an atom, electron rays pass through the atom without absorption. However, as a result of the quantum superposition, electron clouds attract an electron beam without changing their speed and direction. On the periphery where the electron cloud is absent, the rays completely disappear. The intensity of the rays increases in the center, where the thickness of the electron cloud reaches a maximum. As a result, the atom begins to illuminate, depicting its internal construction.

3. Method

The basis of the picoscopy is the electron shifting effect which creates an image of the electron cloud density. At a high resolution of more than 100 pm, the laws of classical mechanics cease to apply but the laws of quantum mechanics begin to work. In time, the law of absorption of the beam by sample (the Beer-Lambert law) on which the operation of the transmission electron microscope is based, ceases to work but the law of the shift of the electron beam (the law of O. Kucherov) begins to work [4].

The Beer–Lambert law relates the attenuation of the plane wave to ***the density of the material*** through which the plane wave is traveling. Then, the intensity is lost, which is a classical mechanical law and, accordingly, the plane wave manifests itself at distances much greater than 100 pm. The Kucherov law relates the local shifting of the plane wave to ***the density of the electron cloud*** through which the plane wave is traveling. The intensity is redistributed at this time. It has a quantum mechanical nature and works at short distances (less than 100 pm). That is, any electron microscope that has a resolution of less than 100 pm becomes a picoscope. At the same time, under the Kucherov law, only the top atom appears in the picoscopy image, no matter how thick the sample is. The transmission electron microscopy then becomes the shifting electron picoscopy. Because, owing to Kucherov's law, it does not measure the absorption of the beam by a sample, but measures the electron cloud density of the individual atom.

4. Material

According to Kucherov's law (1), the illumination intensity of an atom is directly proportional to the number of its electrons. In this way, the picoscopy distinguishes different chemical elements in the same image.

In the Ge/Si(100) system, superlattices are layered structures that contain an interlayer between different materials. All electronics are built on two semiconductors - germanium and silicon. An important task is to study their properties, both separately and in a Ge/Si(100) system. The **s**uperlattice that contains Si cristal, interlayer, and Ge/Si(100) system are obtained by molecular beam epitaxy. The sample was prepared with the method described in [11]. The negative was obtained on a Philips 300 CM transmission electron microscope with an accelerating voltage of 300 kV and a resolution of 140 picometers [12]. The high-resolution transmission electron microscopy in the bright- and dark-field includes the high-angle annular dark field methods. It is important to study weak contrast systems, which is illustrated by the HAADF image of the Ge/Si(100) system. In this case, the thickness d of the epitaxially grown layer is 8700 pm (the Si lattice parameter a100 = 543.07 pm).

As a result, an image of a single atom with all its electrons was obtained for the first time. According to the periodic table, silicon atoms have 14 electrons, which are contained in three shells. Fig. 1 shows the picoscopy image of a silicon atom in Si(010) crystal. This is the first publication of the real structure of a silicon atom. All electrons create a well-organized structure that fully complies with the laws of quantum mechanics. The atom has two pink inner electrons of e11 and e12 in the 1-shell, eight yellow inner electrons e21–e28 in the 2-shell, and four valence electrons e31–e34 in the 3-shell. The two inner shells are formed into two nested spheres of different colors. These spheres are slightly deformed. The external valence electrons form outer surfaces of two types. The electrons e31 and e32 create quantum entanglement with electrons of neighboring atoms. That is, these electrons take part in hybridization and appear as green infinity signs. Electrons e33 and e34 are in unbound active states and look like elongated blue clouds. The right scale of Fig. 1 shows the electron density scale and the distance scale in picometers.

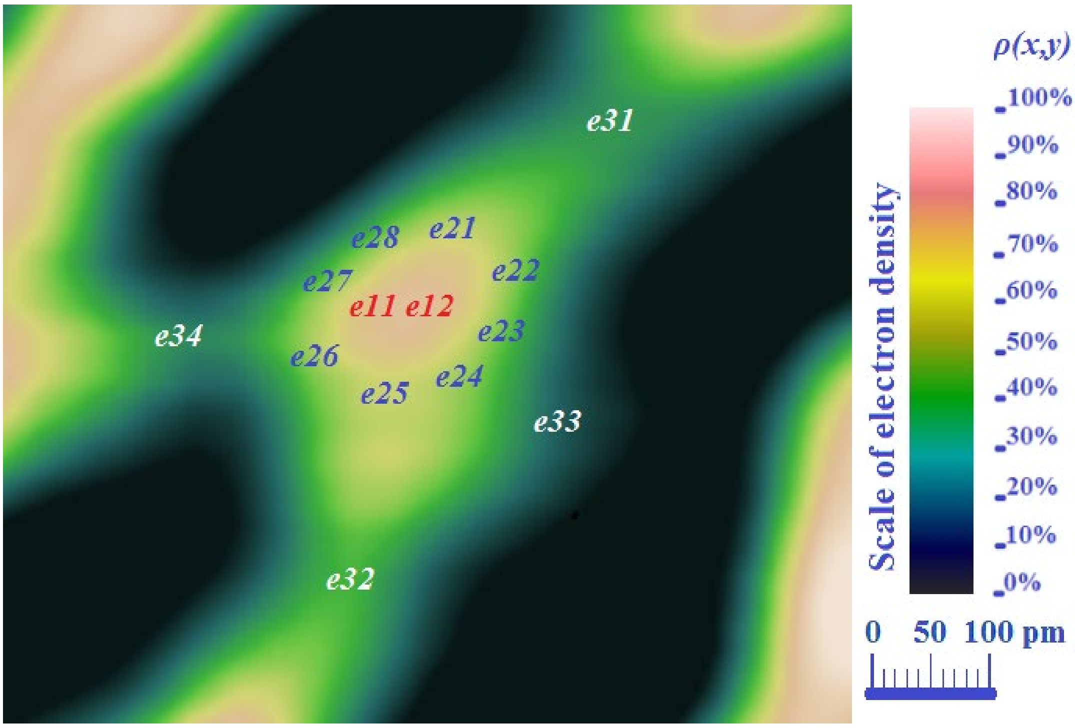

Fig. 1. Picoscopy image of a silicon atom in Si(010) crystal with fourteen electrons: two pink inner electrons e11 and e12 on the 1-shell, eight yellow inner electrons e21–e28 on the 2-shell and four valence electrons e31–e34 on the 3-shell, and valence electrons e31–e34.

5. Visuale Material Science

The picoscopy images of the electron clouds of Ge and Si atoms were obtained with the Kucherov and Lavrovsky method [13, 14] with a resolution of 10 pm.

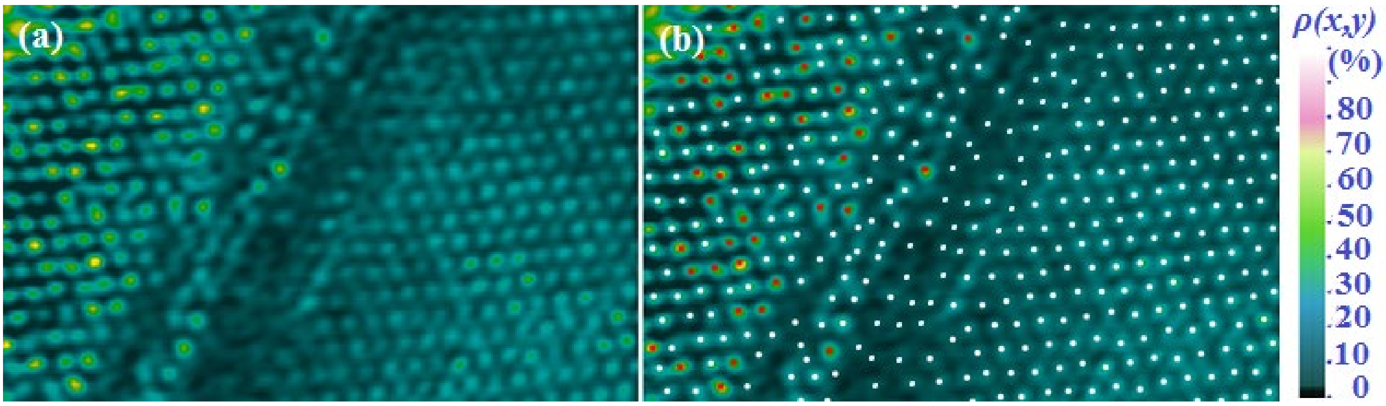

Fig. 2. (**a**) Picoscopy image of a Ge(100) crystal and Ge/Si(100) system and (**b**) An avtomatic atom recognition give Si atoms white and Ge atoms red.

Fig. 2a shows the shifting electron picoscopy image of the Ge(100) crystal (right) and Ge/Si(100) system (left) that contain an interlayer between different materials. Based on the fact that $_{14}$Si atoms have 14 electrons, and $_{32}$Ge atoms have 32 electrons, then, according to formula (1), $_{14}$Si atoms have a blue color (~28%), and $_{32}$Ge atoms have a yellow color (~64%). Thus, picoscopy allows not only to distinguish different chemical elements, but also to measure their position in the periodic table of D.I. Mendeleev. Thus, a method of direct measurement of atomic weight has been obtained. Fig. 2b shows the result of automatic division of atoms into light and dark. The light atoms (germanium) are marked in red, and the white atoms (silicon) are marked in white. In this way, it is the world's first memory device for the computer with cells of atomic size, on the order of 100 pm.

6. Visual Crystallography

It is known that Si has a cubic crystal lattice similar to diamond. However, the picography shows two completely different patterns for these two materials.

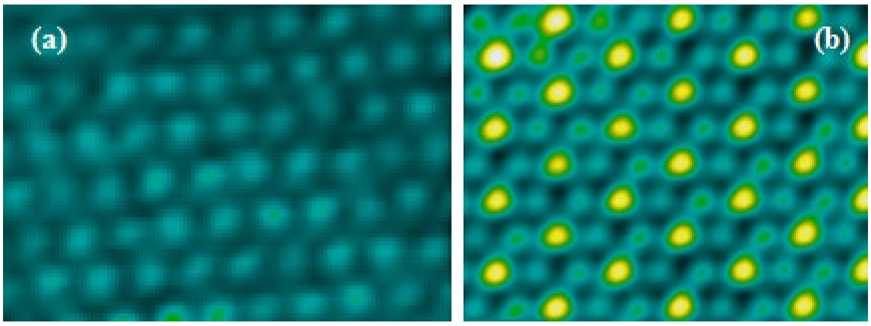

Fig. 3. (**a**) (100) plan of diamond silicon, Si atoms are in the same plane. (**b**) The (100) plan of diamond is corrugated, that is, two-thirds of C atoms are in the plane (blue) and every third carbon atom is above the plane and, therefore, has a yellow color [14].

Crystallography shows that both silicon and diamond have a hexagonal and cubic lattice. Figure 3 shows that in the (100) plan, Si atoms in silicon (Fig. 1a) and C atoms in diamond (Fig. 1b) have the same location. However, the 3D picoscopy shows a significant difference in the structure of these crystals. The Si atoms are in the same plane in silicon (Fig. 1a). While the diamond is corrugated (Fig. 1b), that is, two-thirds of the carbon atoms are in the plane (blue) and every third carbon atom is above the plane and, therefore, has a yellow color [14]. When looking at the crystal lattice of the Si and the Ge/Si(100) system, the crystal lattice of the Si has a cubic diamond structure belonging to the Fd m space group. The atomic occupancy on the (100) plan of Si is displayed in Fig. 4.

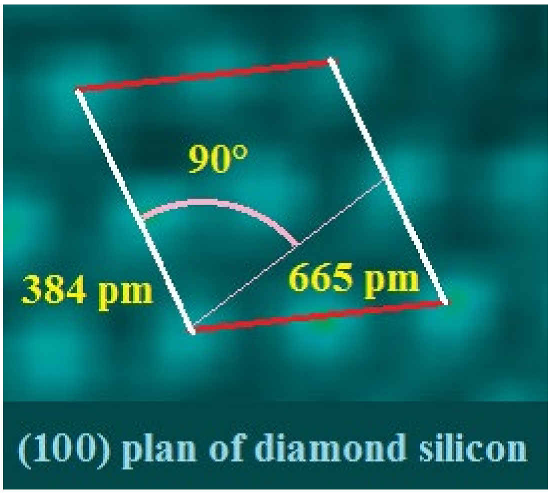

Fig. 4. Lattice structure of diamond silicon [15].

In this scenario, the Si atoms occupy the position as shown in Fig. 1a. White and red lines indicate crystallographic planes (010) and (001). The crystallographic directions are geometric lines linking nodes (centers of atoms) of a crystal. Fig. 3 is part of Fig. 2, and shows the (100) plan in blue in Fig. 5. In Figs. 4 and 5, the (010) and (001) planes are represented by red and white bars, respectively. Figure 5 shows the planes with different Miller indices in cubic crystals.

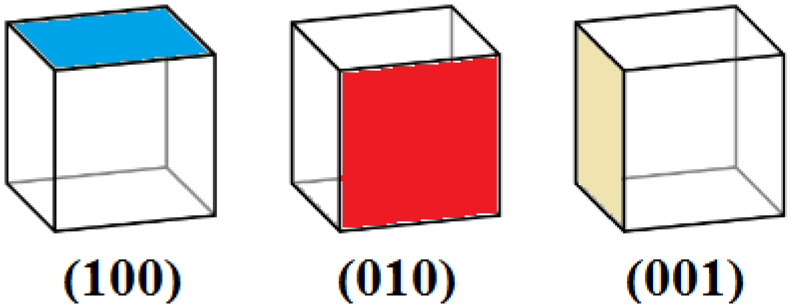

Fig. 5. Planes with different Miller indices in cubic crystals.

The distance between atoms is 384 pm [15]. If we draw lines along the layers of the lattice (Fig. 2), we obtain an ideal single-phase single crystal, and there is no interlayer between the Si crystal and the Ge/Si(100) system.

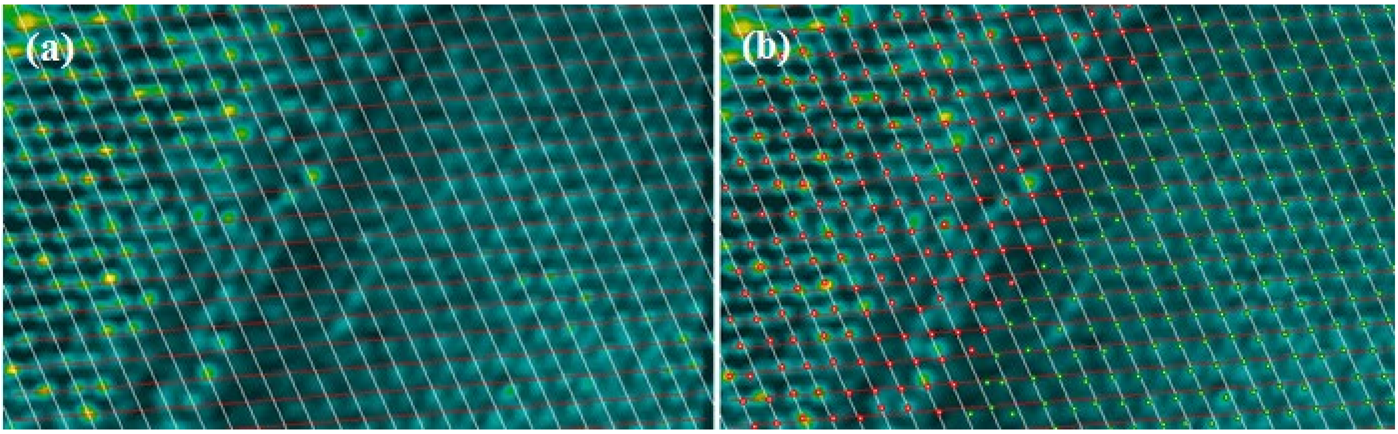

Fig. 5. (**a**) Picoscopy image of the (100) plan of crystalline silicon (**b**) (010) plans are marked with red lines. (001) plans are marked with white lines. Dots mark the real positions of the centers of atoms.

Figure 5a shows the visual crystallography. White and red lines indicate crystallographic planes. An important result is that the crystal lattice of the solution (left) and pure silicon is the same. The (010) plans are marked with red lines, and the (001) plans are marked with white lines.

7. Visible Deformation

Figure 5b shows the deformation of the crystal. Atom centers are marked with dots. The green dots show the centers of atoms in the silicon crystal, and the red dots show the centers of atoms in the solution. The centers of atoms have the maximum intensity of atoms. The position of the atoms is determined with great accuracy as the maximum density of the electron cloud. The error in determining the center of atoms as the intensity maximum is 10 pm.

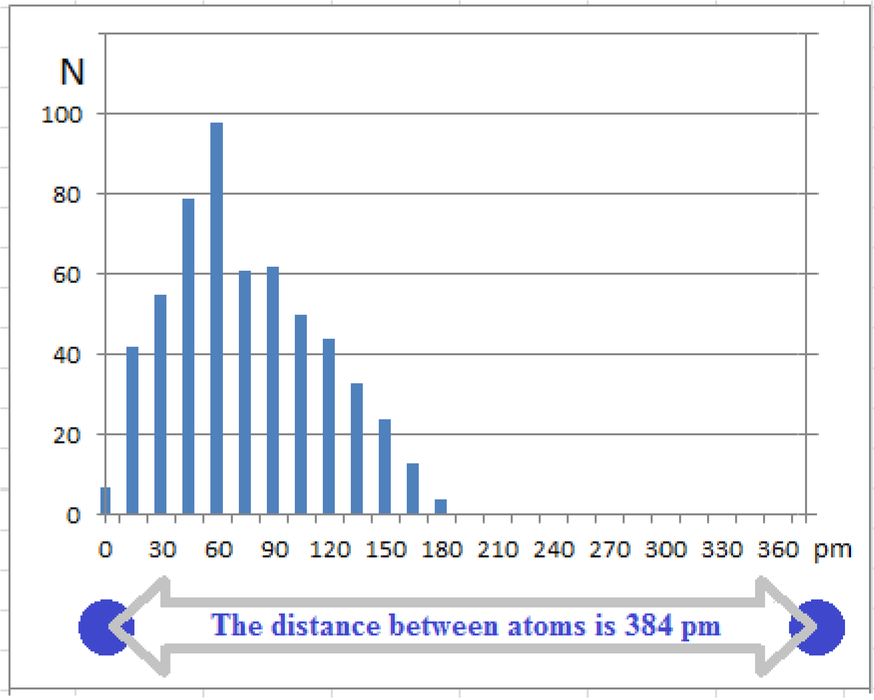

Fig. 6. Histogram of the distribution of the deviation of atoms Si and Ge from the nodes of the crystal lattice.

Fig. 6 shows the deviation statistics of atoms Si and Ge from the nodes in the Si and Ge/Si system crystal lattice. 568 atoms were used in the statistical analysis. The analysis result shows that the deviation is not a stochastic distribution with the center of gravity located at the node. The analysis showed that the nature of the deviation is the deformation of small areas of the crystal. The size of these regions is about the diameters of 10−20 atoms. As shown in the histogram, the average deviation distance is equal to 60 pm, which is 15% of the distance between nodes. This is a direct measurement of the deformation of materials.

8. Interlayer

Superlattices are layered structures that contain an interlayer between different materials. The research confirms the formation of solid solutions Ge(Si) in the Ge film and the Si(Ge) in the Si(100) substrate, which are separated by a thin pseudomorphic interlayer. This strip gave reason to talk about the presence of an interlayer [17,18]. We analyzed the Ge/Si(100) phase composition based on existing literature data and results obtained with the shifting electron picoscopy method. Fig. 1a shows the dark interlayer between the Ge/Si(100) system (left) and the Si(100) crystal (right). However, visible crystallography is shown in Fig. 5b which presents that the Si atoms occupy each lattice point by forming a continuous sequence without any destruction. Namely, the important result is the absence of a layer that separates the base from the solution. That is, the Si crystal passes into the Ge/Si(100) system without obstacles. This proves the absence of an interlayer and correctly interprets the phase composition of the interlayer based on Ge and Si.

9. Conclusions

A Quantum mechanical explanation of the electron cloud densitometry is given in this study. With this effect, an atom begins to illuminate and show its shape. This is the first publication of the real structure of a silicon atom. The atom has two pink inner electrons in the 1-shell, eight yellow inner electrons in the 2-shell, and four valence electrons in the 3-shell. The electron cloud densitometry image shows Si atoms in blue and Ge atoms in yellow. By measuring the density of the electron cloud, a technology for distinguishing atoms has been developed. Studying emission from Ge/Si(100) system, having a non-monotonous character, is of high interest for creating picoelectronic devices based on new atomic size memory cells. As a result, visual crystallography becomes a new branch of applied functional materials.

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Conflicts of Interest: The author declares no conflict of interest.

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