Seeking stronger steel, systematic look at 120 combinations of alloy elements provides clues

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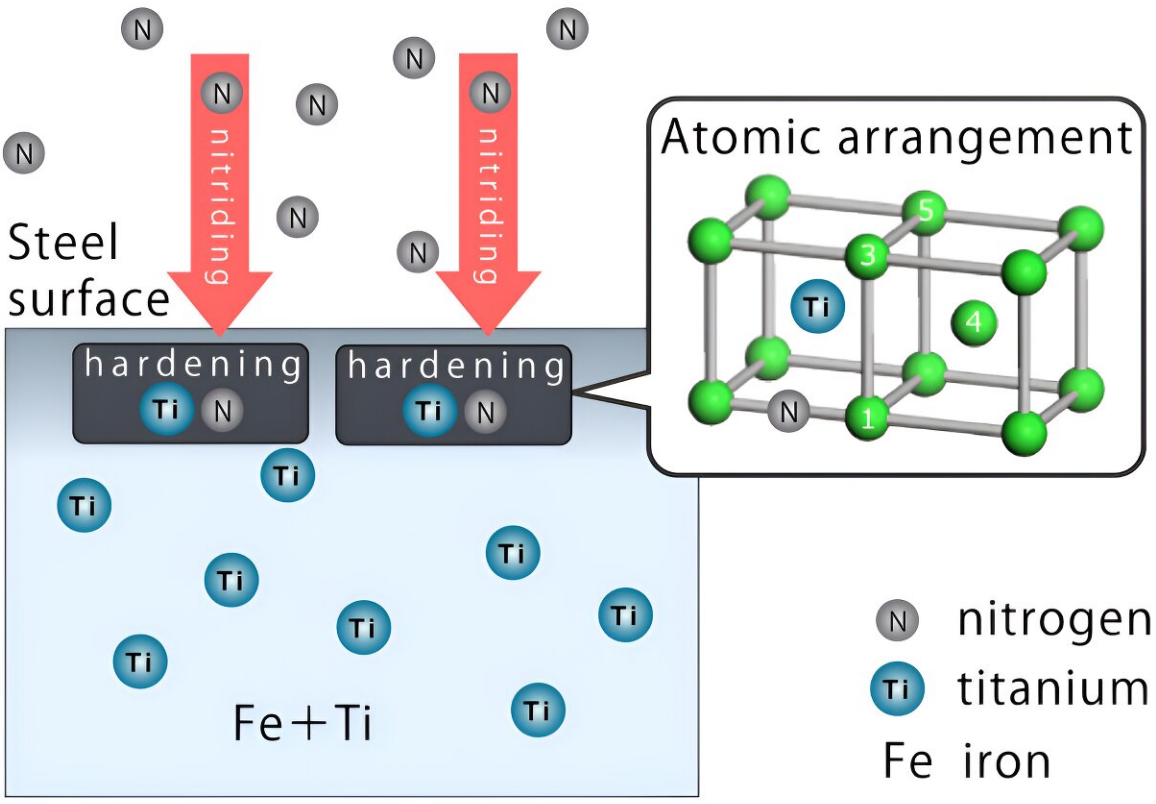

Model of stable configuration of nitrogen and titanium in steel of iron-titanium alloy. Credit: Osaka Metropolitan University

Decarbonization of automobiles not only requires a shift from gasoline

engines to electric motors, but also quality steel parts that help the motors run while lessening the weight of vehicles. High-performance steel materials can offer quieter rides and resist the wear and tear from high-speed rotation in motors. To create them, the process of modifying the steel surface with carbon, nitrogen, and alloy elements needs to be optimized.

To understand the interactions between elements in steel, a systematic investigation has been conducted by an Osaka Metropolitan University research group led by Associate Professor Tokuteru Uesugi of the Graduate School of Informatics. The group theoretically calculated 120 combinations of how 12 alloy elements, including aluminum and titanium, interact with carbon during carburization and nitrogen in the nitriding process.

The findings were published in *ISIJ International*.

The results showed that when titanium is placed in a specific arrangement, it bonds with nitrogen or carbon, hardening the iron. The group's analytical data also showed that the alloy element must have a larger metallic radius than the iron atom to bond well.

"Although it was not easy to elucidate the mechanism from the results of numerous calculations, we used multiple linear regression and stratified analysis through trial and error," Professor Uesugi stated. "These results are expected to contribute to a better understanding of the mechanisms of steel strengthening and improved durability, and to the development of superior materials."

More information: Tokuteru Uesugi et al, Interactions between Interstitial and Substitutional Elements of Solute Diatomic and

Triatomic Clusters in α-Fe from First-principles Calculations, *ISIJ International* (2024). DOI: 10.2355/isijinternational.ISIJINT-2024-062