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RAFAEL JARAMILLO: All right, good morning, everybody. Today is not a thermodynamics lecture by me. We have a guest lecture by Professor Greg Olson. And we just finished a lot of work with thermocalc, and CALPHAD, in general, and solution modeling, and binary phase diagrams. And I've told you throughout the entire semester that thermodynamic data is valuable and allows you to make predictions. That's why it's valuable, and those predictions allow you to make real things in the real world possible.

And so far, you've just had to take my word for it. So the point of today's guest lecture is that so you don't have to take my word for it anymore. So I'll just say that Professor Olson is world famous for using thermodynamic data for real-world impact. And I leave it at that. Is that OK, Greg?

GREG OLSON: That's sufficient, I think. Yes. Let's hope it's positive impact, yes. OK, very good.

RAFAEL JARAMILLO: So I'll hand it over to you.

GREG OLSON: All right. Let me attempt my screen share. All right, my presentation will be from the perspective of my university day job, as well as the activities of our computational materials design company, QuesTek, and their ongoing collaborations through the Chicago-based CHIMaD materials design center. As thermocalc professor of the practice, my job description is to make MIT a global beacon of CALPHAD technology, into which we are recruiting you.

And in support of that, we've actually had a range that MIT would host this year's international CALPHAD conference. But unfortunately, due to the pandemic, we've had to postpone it a couple of years. But I hope you'll still be around to join us when that happens.

And I would like you, throughout, don't hesitate to interrupt. Just unmute yourself, and yell at me, if you'd like to discuss anything.

The context of this technology is the National Materials Genome Initiative-- that's a presidential initiative announced by President Obama a decade ago, intended as a decadal initiative, but in fact, a recent National Academy study has recommended that it continue for another decade. And the overarching goal of this initiative is to build out the databases and tools that would allow us to take what has been historically a 10 to 20-year materials development cycle and compress that by at least 50%.

The metaphor of the genome is discussed in the National Academy study going back to 2004, on this very subject of accelerating the technology transition of materials and processes. So it reviewed the best that had been achieved at that time. And then, looking forward, looked at the analogy of the Human Genome Initiative as possibly the greatest engineering database in history that was created not just to support the life sciences, but really to support science-based medicine-- an example of which is that mRNA vaccine we're all getting these days. So it's had a tremendous impact in allowing a more science-based approach to medicine.

So the concept of the materials genome from the start, as called for in this 2004 study, was to build out an equally fundamental database, with the idea that the human genome physically functions as a database that directs the assembly of the structures of life. What are the equally fundamental parameters that direct the assembly of the microstructure of materials, and could we use such a system to not just support material science, but to enable a new form of science-based materials engineering?

So it really was the ultimate engineering application, and the ability to put our scientific understanding in a useful predictive form-- that really was the central concept of this Materials Genome Initiative. And the recommendation in 2004 is exactly the structure that was formed, and then is continuing today.

Now, there have been many Academy studies acknowledging the new opportunity of computational materials engineering, but one thing that was unique about the 2004 study was the leading role of global network of small businesses that created and maintained this technology and made this possible.

And so this was a list that was constructed in that report of what had already been made available at that time, and demonstrated successes of the technology. The principle mechanism by the way that this technology has moved into major corporations has been by acquisitions of various forms that have affected about a third of the companies on this chart.

So small business really did create this technology and lead the way.

Historic milestone was a decade ago with the first flight of QuesTek's ferrium S53 stainless landing gear steel. And this was the first stainless steel to meet the mechanical performance requirements of aircraft landing gear, which was driven by the need to eliminate toxic cadmium plating. So this was a green steel, solving an environmental issue.

But more significant, it represented the first fully computationally designed and flight-qualified material to go all the way to flight. And that was just in December of 2010. So that really measures a high level of maturity of this technology even before the National MGI was created.

And that is reinforced by this timeline. So there had been debate as to what a materials genome could be-- it's very clear the genome we have is, in fact, the CALPHAD database system, whose origins go back to Kaufman and Cohen at MIT in the 1950s, with the calculation of the iron nickel phase diagram.

I'd like to emphasize, though, the CALPHAD acronym is based on calculation of phase diagrams, but the reason for that acronym was to distinguish it from something called PHACOMP at the time, that was a technique that was trying to estimate solubility limits in alloys from the attributes of a single phase. And CALPHAD acknowledges that solubility is really based on phase competition that is represented by phase diagrams in the equilibrium limit.

But in fact, I think, yes--

RAFAEL JARAMILLO: If you don't mind, can you just briefly tell us about landing gear, and why that's such an accomplishment? I think we take a lot of these things for granted. What is it-- if there's one of many material criteria, for instance, that makes it such a demanding application, so we can understand why that's such a big deal.

GREG OLSON: Yeah, I think I'll come back to it a bit later. But it is-- the big challenge is that the high chromium levels that you need to get the corrosion resistance are in conflict with the things you need for the mechanical performance of strength and fracture toughness. And it was a matter of using a predictive science approach to take it to a higher level of optimization that could resolve that conflict. That wasn't going to happen by empirical development. Yeah.

And I'll illustrate what was key to that later on. But I want to emphasize that, actually, is the name of your class materials at equilibrium, still? Is that the name that's used?

RAFAEL JARAMILLO: No, it's thermodynamics, but it might as well be materials at equilibrium.

GREG OLSON: OK, all right. Because we tend to think of-- I think the way thermodynamics is taught often, we tend to think of it as something that applies only to equilibrium. But the truth is, it wouldn't be called thermodynamics if it was only about equilibrium. It was created to describe heat engines that are highly dynamic systems, where in modeling them, it was useful to look at equilibrium limits.

It's also very useful, if you want to measure thermodynamics, we should take systems to equilibrium. So we know what we're measuring. But really, the power of thermodynamics is it describes the driving force of dynamic systems. And it really drives the evolution of microstructures and processing and service.

So it really is, in that sense, the genomic data that drives the systems.

So in fact, I prefer to describe CALPHAD as calculated phase dynamics. And so it starts with thermodynamics, but it's real power system is far from equilibrium. And in fact, when it was invented by Kaufman and Cohen, what they were really trying to do was not to calculate a phase diagram, they were trying to take the information that's there in an equilibrium diagram and reduce it to its underlying thermodynamics, so they could apply that thermodynamics to martensitic transformations that are far from equilibrium.

So it was really to create-- get the underlying thermodynamics to understand the driving forces for the dynamics of martensitic transformations. So it really is the non-equilibrium applications that drove the creation of the technology in the first place. So it began as solution thermodynamics, and became an international organization in the 1970s.

And the first commercial software showed up around the 1980s. But then, it expanded from solution thermodynamics to adding mobility databases, and solving multi-component diffusion problems, moving on to other phase-level attributes, such as elastic constants. So an increasing array of phase-level thermodynamic and kinetic attributes over an expanding scope of materials, from metals to ceramics. And very recently, organic systems, as well.

All of which was largely based on empirical measurement. But today, DFT physics calculations have received enough accuracy and efficiency that they now actually actively participate, and we integrate into the assessment of these databases the predictions from physics calculations-- at least for 0 Kelvin, the enthalpy predictions.

So it was the arrival of the thermal system as a commercial code, and a supporting software database structure set by the European SGTE consortium that set some level of standardization, that really inspired our founding in 1985 of our SRG design consortium. And this was founded at MIT.

And the idea was to create a general methodology of computational materials design that would be enabled by these underlying CALPHAD databases. With the idea that we would use high performance steel as the first example, acknowledging that we studied steel the longest, have the deepest predictive science foundation in steel. And also, at that point, the highest quality of thermodynamic data was available for steels-- to use that as the demonstrator.

So our first projects were designs of steels. But throughout the 1990s, we did a number of demo projects that applied the same methodology to other alloy systems, polymers, ceramics, and even some composites, to show its generality. And it was the first steel designs that ultimately led to the founding in the late 1990s of QuesTek as a company that could offer computational design services based on this technology.

But what the CALPHAD is really allowing us to do is use this mechanistic understanding we already possess, but use it in a quantitative system-specific way. And that's what enabled the successful demonstrations of design of new materials throughout the 1990s. And it was largely that demonstrated success that made the case for the DARPA AIM initiative, which began at the start of the new millennium.

And this was really addressing the central focus of what is now the MGI, and what we now call integrated computational materials engineering, or ICME. And this was to go beyond the design of an alloy, and set a specification of composition and process temperatures to really address the full materials development cycle.

And this meant connecting materials models to macroscopic process models to handle material production scale-up, process optimization at the component level of things like landing gear. And then, most important, the forecast of manufacturing variation, so that you could predict the minimum properties of a material that a user could count on, at a 1% probability basis. And that's what it takes to get a material actually flight-qualified for critical applications.

So at this point, we've had over six decades of building out a materials genome with CALPHAD structure. About 30 years now of a full design technology, and we've now been at 20 years of a fully integrated process. So it's quite developed. And as I'll touch on later on, what this has allowed the compression of the materials development cycle, getting it down to the cycle of product development, has allowed for the first time to include materials in concurrent engineering.

Historically concurrent engineering meant everything but materials-- you had to use whatever materials were available. And now, there are a number of success stories I'll touch on later, where materials have been fully integrated in concurrency, and allowing a very strong synergy between materials development and product development. So that's the landscape.

Core of our approach is the philosophy of the late great Cyril Stanley Smith of MIT, who looked at the general principles of dynamic, interactive, multilevel structure, or structure hierarchy, and acknowledged an intrinsic complexity of material structure. For which he advocated that we should be taking a systems approach. And essentially, using the same framework of systems engineering that the rest of engineering is already using.

So we've taken that to heart. And to implement it, another important contribution from the late great Maurice Cohen of MIT, is what he described as a reciprocity between the opposite philosophies of science and engineering that are represented by this unique linear structure, in which the predictive cause and effect logic of science flows from left to right. And the inductive goals means logic of engineering flows from right to left.

So it actually allows us to bring these two philosophies together in a streamlined, non-turbulent way. So the scientific prediction is that however we process a material will determine its structure, the structure will determine the properties, and the combination of properties will determine its performance.

And this, then, enables a design system where we can set performance goals for a new material that we map to a set of property objectives, use our knowledge of structure property relations to devise possible microstructures that are accessible through prescribed processing.

It's important to know that the flow from left to right is unique. That exactly how we process will determine that structure and its unique set of properties and performance. It's always the nature of this inverse problem that we do not have uniqueness. That once we have a set of property objectives, there are multiple structures, and multiple process pathways that we could use to achieve it.

So the approach in adopting a system framework is to use this as the backbone of a system structure and add Smith's structural hierarchy to it. So that each design project starts with a system chart. And the idea here is to get the entire material down on a page.

So the left to right flow of this is the cause and effect logic, but the process of design works from right to left, where performance goals overall will be mapped to a quantitative set of properties, such as strength, toughness for high performance steel, and resistance to environmental hydrogen enbrittlement.

And from our mechanistic knowledge, we know that those properties map back to different subsystems in the hierarchy of microstructural subsystems, which we know dynamically evolve throughout the stages of materials processing. And that allows us to, then, identify and prioritize the key structure property links and process structure links for which we want to build out our design models.

Now, that can be done by empirical correlations that are useful for interpolation. But we really, from the start, were committed to getting the most value out of the CALPHAD fundamental data, is to use predictive science based on mechanistic understanding, and to express that mechanistic under form that we could parameterize to devise parameters accessible to those fundamental databases to make a quantitative approach to the full design of the material that produces different levels of microstructure throughout different stages of processing. And meets all those property requirements for useful material.

And what that motivated was the models summarized here, which really is a subset of what's available in computational material science that allowed us to do quantitative engineering. So at the bottom level, the three fields we integrated were the DFT physics that was particularly useful for surface thermodynamics, which is more difficult to measure than bulk thermodynamics. And of course, the material science is particularly advanced in the theory of solid state precipitation, and precipitation strengthening.

And for structure property relations, we applied-- brought in the micromechanical applications of continuum mechanics to simulate unit processes of fracture and fatigue, to set the structure property relations. So these are really the three disciplines that were integrated in this approach to meet performance goals.

But equally important is to constrain the process ability of a material, and that's a role for the CALPHAD-based material science models of the solid-solid phase transformations, and the liquid-solid phase transformations. Both of which are scale dependent, in terms of the size of heat-treated components through the size dependence of heat transfer.

So ultimately, it's the linking of these microstructural models to the macroscopic process simulations that allow us to constrain materials up front, theoretically, to be processible on a desired scale. And that really helps to accelerate the full cycle, instead of experimental scale-up.

So what's represented here on the right are the software models and their platforms. And the advanced instrumentation is equally important-- the ability to use techniques, such as the atom probe, to actually measure the complex compositions of nanoscale strengthening precipitates in our ultra high-strength materials.

So from the start, calibration and validation to understand the associated uncertainty of our predictions was really important. And that's what the instrumentation was enabled.

So a first example-- starting out in the 1980s, to design ultra high-strength steels, we first took apart the highest performance steel of the time, which was the AF1410 steel, which is tempered at 510C, to precipitate alloy M2C carbide. So these are HCP carbides, where the M is a combination of chromium, molybdenum, and vanadium, and sometimes tungsten.

So we brought together a wide array of techniques that map the time evolution of the precipitate particle size, the aspect ratio of the carbide, their number density, total volume fraction, and the evolution of the carbide lattice parameters and associated composition trajectory. And then, this summarizes the evolution of the precipitation strengthening.

The evolution of the size was consistent with the theory of precipitation at high super saturations. And in that regime, we can treat the initial, critical nucleus size as the fundamental scaling factor for particle size that's so important to strengthening. And that, of course, scales inversely with the precipitation driving force. So this is a way we could get a thermodynamic handle on the particle size that governs strengthening efficiency in these systems.

But it was important to recognize that the trajectory of the lattice parameters, driven by the composition trajectory of the carbides, is consistent with the initial nucleation being in a fully coherent state. So it was necessary to add to the CALPHAD chemical thermodynamics an elastic energy term, that's composition-dependent through the composition dependence of the lattice parameters, setting the misfit strings.

So all that was put together to get a precise driving forces for the precipitation of these carbides, so we could efficiently control the particle size. And what that leads to, then, is this simplified parametric approach to strengthening, where from the Orelon strengthening theory, the precipitation strengthening scales inversely with the spacing of the obstacles, and that spacing scales with particle size over phase fraction to the one half, for the spacing in a slip plane.

And that means, then, the precipitation strengthening goes as f to the 1/2 over particle size. And if we accept this scaling to the initial critical nucleus size that scales inversely to the driving force, then we can write that the precipitation strengthening will scale directly with that thermodynamic driving force, times phase fraction to the 1/2.

So this predicted that we ought to be able to design steels with higher driving forces to get more efficient strengthening. And that was then tested by making a series of steels that had a fixed carbon content, setting the ultimate phase fraction of the precipitates. And then, we used our coherent thermodynamics to predict the driving force.

But as well, by the time we get to the temperatures where we can have substitutional diffusion, the carbon diffusion controlled formation of iron carbide, like FE3C will already have occurred. And that lowers the chemical potential of the carbon. So it was necessary to get these driving forces right. We had to first consider a constrained equilibrium with FE3C to set the carbon potential.

And then, we were able to validate that within the scatter of these measurements, at a fixed carbon level, we could vary the hardness, peak hardness of this strength and steel, over about 20 points on a Rockwell C scale. So very dramatic, direct proportionality predicted by the model.

And so that calibration became the principal tool that we used to design steels with much more efficient strengthening, demonstrating alloys that, for a given carbon content, could have 50% more strength than the previous technology. So it's an area that's been highly developed empirically, but in fact, there was a lot more to be achieved by being more predictive and taking systems to a high level of optimization using these tools.

Now, what I wanted to just touch on is there's also an important role of the surface thermodynamics. And this is a case where we made very good use of the DFT predictions. But what this chart is about is a correlation of the embrittlement potency of interfacial segregates against the segregation energy difference between free surfaces and grain boundaries. And in this case, there is experimental data to validate this, but this is actually the case of predicting it with our DFT quantum mechanics, with pretty good accuracy.

So these are the well-known interstitial components that have been well-studied. Substitutional elements are less well-studied. So after demonstrating the ability to compute these numbers, we actually built out this database of the embrittlement potency from surface thermodynamics, which was calibrated and validated by some large-scale DFT calculations, giving us these predictions, from which we were able to identify the strong cohesion enhancers that could sufficiently enhance grain boundary cohesion to offset the embrittling effect of hydrogen.

And this allowed us to design these very high-performance steels to no longer be prone to the intergranular form of stress corrosion cracking. So it was a big advance in the resistance to hydrogen embrittlement in this class of steels. So it's one example-- yeah?

RAFAEL JARAMILLO: One thing, can you fill in what is DFT? We've heard it several times this point. We talk about data a lot, so where does that data come from?

GREG OLSON: Yeah, so that's density functional theory. So so this is something that we basically have ways to solve the Schrodinger equation. But there is a menu of approximations that you do take along the way. But it really is essentially first principles prediction of energy at 0 Kelvin.

RAFAEL JARAMILLO: So we use a lot of empirical data, in 020, but you've also probably used DFT-derived data, even without knowing it. So when you have some materials property data, that comes from somewhere, and sometimes it comes from theory, and sometimes it comes from measurement.

And oftentimes if it comes from theory, it comes from DFT calculations.

GREG OLSON: Yeah, it is. And there are different approximations, and this was an all-electron method, very rigorous. But it was typically something like 400 hours of Cray supercomputer time for each data point, back in the 1980s, when we did that.

RAFAEL JARAMILLO: And I'll just chime in-- Ali asked a question, which do you prefer? I think you mean, which do you prefer, experiment or theory?

Is that what you meant, Ali? Speak up-- unmute yourself. It's more fun.

STUDENT: Yeah, I mean like for the applications like of prediction, which is better to extrapolate?

RAFAEL JARAMILLO: Greg, if you had your choice-- I mean, I'll just say, first of all, it's often not-- it's often an apples to oranges comparison. Because we use DFT most often to get data for processes or situations that we just can't measure. Which I think gives you your answer. If you have apples to apples, if you have a measurement and calculation of the same thing in the same circumstance, I think Greg and I would agree, if the measurement is a good one, we'd go with that.

GREG OLSON: Yeah, if you look at the magnitude of this, we're using this method to find the ones that have this cohesion-enhancing potency of greater than 1 EV. And the intrinsic uncertainty of even these calculations is about 0.1 EV. And this other model got it within 0.2 EV.

So it is important to understand the uncertainty of those predictions. So if it's plus or 0.1 EV, that's fine for helping you find the 1 EV candidates. But most often in metallurgy, the number we want to know is only of the magnitude 0.1, and 0.1 plus or 0.1 is not very useful. So it's a good way to find out where to go for the big numbers, but most of the time, we really need the experimental data that gives us higher accuracy than we can get currently from the DFT methods.

So that's why I was saying, that up front, uncertainty quantification was a very important part of the whole strategy of putting these tools together.

But this is a good example of maximum use of DFT-- we had a small set of experimental surface thermodynamics to test against. And then, we could calibrate against the ability of DFT to predict it. And then, make this projection across the periodic table. So it's a surface thermodynamic genome almost entirely from DFT calculations.

And the way we put it all together is graphical parametric design. So we map the behaviors of interest back to these parameters, like driving force and phase fraction for strengthening. And so for the actual stainless landing gear steel, here's a cross-plot versus molybdenum content affecting the driving force and the carbon affecting the phase fraction. And there are a couple invisible yellow contours showing how the driving force increases with molybdenum, and of course, the carbon sets the phase fraction, so it's this region in here that gave us the strength level that is our goal for the design.

And superimposed on that, our process ability constraints, such as the martensite start temperature, to have a fully martensitic steel. And the solution temperature to put the reactive components in solution so we can precipitate them at high temperatures.

And the relative slopes that we can see from these types of plots also allow us to assess relative sensitivities, so we can develop robust design strategies that don't require too tight a tolerance.

So quite typically, we start from the last stage of processing the nanoscale precipitation that meets the strength goals. And then, back up to earlier stages of processing, where we're also using these FCC MC type carbides. In this case, we've got a composition variable in the process temperature. So we're constraining these grain-refining particles to be soluble at homogenization temperatures, able to precipitate out at forging temperatures, and then maintain a certain phase fraction in size at the final austenitizing temperature of the steel that sets the grain size of the steel.

So similarly, we can back up to even earlier stages of processing, specify the de-oxidation processes that set the primary inclusions at the multi-micron level that are important to toughness and fatigue resistance.

But that graphical strategy is very efficient, and it is the practice that we use at QuesTek and the practice that I teach in my design class.

So the first four products to come out of that are these high-performance secondary hardening steels. We have now two flight-qualified steels, as well as the stainless that's used by the Air Force. We have a high toughness steel that's first gone into the hook shank application for the carrier-based planes. So both of those steels are flying.

We also have very high performance carburizing steels for gear steels for fatigue resistance, and that's doing well on off-road and on-track racing. And in fact, the Red Bull Formula One team that's very competitive this year is actually using our gear steels for their reliability. And those gear steels now are being qualified for helicopter applications.

But all of these benefit from that extra strengthening efficiency that we get by refining those M2C carbides down to a 3-nanometer size scale through that maximization of driving force, as validated here by an early 3D atom probe reconstruction.

So all four of those steels are using greater strengthening efficiency to resolve the conflict with other properties.

RAFAEL JARAMILLO: This is maybe the second or third time you've mentioned atom probe, and there's a data set right in the middle here. So it seems like a good opportunity to talk about what that is.

GREG OLSON: Yes, the atom probe is a version of the field ion microscope that looks at the point of a very sharp pin to get very high electric fields. And it can actually cause evaporation from the high fields. And so we can evaporate atoms off of the tip, and project them to a position-sensitive detector, and actually reconstruct the position of the atoms in the tip. So it really is taking us down to a nanoscale spatial resolution with detectability of all atoms in the periodic table. So a very powerful technique.

RAFAEL JARAMILLO: If I may, it pulls apart a material, atom by atom, and tells you where all the atoms were.

GREG OLSON: Yep, that's what it does. Yes.

And we have very good facility at Northwestern, but there's also a very good one at Harvard that we're using now.

STUDENT: Can you use the material after that? Does it change the surface?

GREG OLSON: Yeah, this is true tomography. So we're fully-- we are really toning the material and taking it apart. But one thing we can do is, before we do the tomography, we can look at the tip in the electron microscope. So we can get diffraction information, crystallographic data, fully characterize the tip into EM before we then take it apart in the atom probe.

RAFAEL JARAMILLO: But it does-- it's like getting beamed up, but you're never getting beamed back down.

GREG OLSON: That's right.

RAFAEL JARAMILLO: It tears the material apart atom by atom, and does not put it back together again.

GREG OLSON: Right. Well, it puts it back together theoretically, right. Yeah, so we reassemble it as tomography. Yep.

All right, yeah, I would just touch on the DARPA AIM initiative. Again, this full compression of the cycle is this linking to macroscopic process models. And so we were able to work with GE and Pratt and Whitney, and learn about the technology of multidisciplinary computational engineering. So this integrator was linked to the tools of macroscopic aero-turbine engine design, including heat transfer for heat treatment.

So we built this PrecipiCalc simulator. So this puts together the CALPHAD thermo and mobility databases, and adds some surface thermodynamic quantities to actually simulate complex nucleation and growth in complex alloys, so that we could actually predict the effects of very complex heat treatments of turbine disks that had multimodal distributions of gamma prime precipitates. And very accurately control it, and use it to demonstrate it, and process optimization. Validating predicted overspeed burst speed of a turbine disk.

And then, ultimately, we did develop strategies to predict the cumulative probability distribution of properties from the variation that can occur during manufacturing from the allowed tolerances of the specifications of material composition and processing. And we were able to get information that normally would take a lot of time and money, and a lot of testing, like 300 turbine disks, before you'd have enough data.

And we could, with only 15 data points, and mechanistic models, actually predict this 1% minimum property at room temperature and elevated temperature. So we demonstrated the strategy to get the qualification data of necessary minimum properties very efficiently by predictive modeling based on these CALPHAD tools.

And so here's the time chart on the two landing gear steels. So this is the technology readiness levels at the level of the landing gear. Here's the corresponding materials milestones. And so both of these steels went from a clean sheet of paper to flight in less than a decade-- meeting the MGI goals.

But particularly doing it the second time, we were able to move more quickly into the Navy trusting our predictions well enough to give us the technology for the hook shank application. So we actually had component qualification within a month of material qualification, in that case.

And this has been a case study for the MGI program, where it was reviewed in the second landing gear steel-- what were the technology accelerators using this technology? And what were the inhibitors doing it in a small business where there were lapses in the federal funding of the projects, and there was a reliance on toll manufacturing by others?

It was estimated that we had really demonstrated a technology capable of a three-year cycle. And that's really the important key of that's what enables concurrency. And really, the most historic example of that so far was the Apple Watch announced in 2014.

So these are all new alloys developed by Apple that were designed and developed concurrently with the development of this device. And actually, delivered in less than two years from their acquiring the technology from QuesTek to actually do this. And that included the high strength anodizable aluminum alloy that ultimately went into the 6S iPhone.

So it's been estimated there's now a 50% chance that you've got a computationally designed material in your pocket. And it came from this CALPHAD-based technology.

From there, news travels fast in the Valley, and it caught the attention of this guy. I actually had the opportunity-- he invited me out to give him a half-hour elevator pitch. I thought I was selling him our technology, it turns out I was selling him Charlie Cumin, my former student who was the founding president and CEO who had gone to Apple.

And so after three years at Apple, he moved to be vice president of materials technology at both SpaceX and Tesla. So this technology has been taken even further in that environment. And notably, included a burn-resistant nickel super alloy that allows the high oxygen pressures that really enables the Raptor engine of the Mars Starship.

So it gives you a rare example of a corporate CEO bragging about his metallurgies.

I think what I'll do is I just want to mention back here on planet Earth, we've got this CHIMaD center as a decadal center supporting the MGI. It's in its second five years of its 10 years. It's largely based in Chicago, but MIT is a partner to it. And it's looking at not only improving these methodologies, but greatly expanding their scope. Notably, including taking this to organic systems and polymers, as well, and they're building out essentially a polymer CALPHAD to design all materials by the same methodology.

And I'll just mention that a lot of the current projects are looking specifically at the design of materials for the new technology of additive manufacturing. And here's some of the early projects at QuesTek in that field. And one of our more important designs was a high-temperature aluminum that uses unique features of additive manufacturing, that compared to this scandium bearing alloy, we have scandium-free alloys using some rare Earth elements, that are able to sustain high strength in aluminum alloy out to very high temperatures.

Very promising. And it's a unique microstructure that can only be achieved by additive manufacturing.

I did want to mention electroceramic-- we had the opportunity under this DARPA Simplex program-- we were asked by DARPA to look at integrating new data-mining techniques with our CALPHAD-based design strategy, and apply it specifically to thermoelectric systems.

So here, this is the system chart for a thermoelectric material, where the basic conflict is we want electrical conductivity, but not thermal conductivity. And the way to break that is to use microstructure for phonon scattering to get the thermal conductivity down.

So it was a chance to use the same kind of hierarchical microstructures that we use in structural alloys of precipitation and grain refinement to manage the thermal conductivity. And one early example of that was to build out the CALPHAD thermodynamics of this lead telluride, lead sulfide system, taking the same framework. And then, actually, predict from a phonon scattering model-- if we optimize the particle size, what level of performance we could achieve as we vary the phase fraction of the lead sulfide particles.

And it showed that it agreed with the data from empirical development, the literature, at low phase fractions. But actually said at these higher phase fractions, if we were to refine the particles to their optimum size, there is more performance that you could achieve from that system. So this is a very early demo of applying CALPHAD to these systems, as well.

And this is underway now as part of the CHIMaD center, Jeff Snyder at Northwestern is actively developing the use of the CALPHAD to control-- predictably control microstructure optimization in these same systems.

But of course, what you really want to know is, what about bubble gum? And so we did get support from Wrigley-- did have four years of support for a doctor of bubblegum. And we were asked to make a four-component, easy-to-manufacture gum, similar to Hubba Bubba Seriously Strawberry, could we, with that simple a formula, get the performance level of Hubba Bubba Max-- which is the highest performance commercial bubble gum, but very difficult to manufacture.

And we did succeed with our modeling to even outperform the highest performance gum out there. So we finally had produced a material that society could appreciate. It was very rewarding.

And this was aided by a student team that actually won the ASM design competition back in 2008. And if you'd like to learn more about that, I suggest you sign up next year for 3041 and learn how to be a materials designer. Here's an example of the five projects currently underway. All of these connect back to the CHIMaD research.

So the teams identified in red here are all being coached by doctoral students, and post-docs, whose thesis is on that particular design project, to help student teams get to the high technical level it takes to actually do the computational design of a complete material with some challenging objectives.

Notably, including a project this year where Apple is the client. And we've had a number of students coming out of the class who have gone to take internships over the summer at Apple. They're very pleased with the students.

So I highly recommend you sign up and join us next year.

RAFAEL JARAMILLO: All right. Well, that was fantastic. That covered a lot of ground, Greg. And we're right on time.

GREG OLSON: I hope it wasn't too dizzying, but of course, you have the opportunity to go back and play it over it slow me down.

RAFAEL JARAMILLO: It was dizzying, but it was a really impressive show of impact. So thank you.

We have-- so as usual, I'm going to stop recording in a minute. But I'm very happy to take questions. I'm sure Greg is happy to take questions for a couple of minutes.

GREG OLSON: Indeed.

RAFAEL JARAMILLO: --till the bottom of the hour. No? Questions about CALPHAD, the mechanism, the history, the science, landing gear, Elon Musk? Any of the above, I'm sure.

Did you know how important this was to your-- well, to your modern lives?

GREG OLSON: Even in your iPhone. And it will help reduce-- it will help reduce the price of your Mars ticket, too, the efficiency of the engine.

STUDENT: Of the models that worked with the heat-- that worked with the heat transfer from other companies, I think you said you're working with the-- I don't know if it's Air Force or DARPA, that you've collaborated with other engineering companies?

GREG OLSON: Yeah, so right, so the idea of ICME is to link the materials models to the macroscopic processing tools, where very often, it's all about the heat transfer. So we were in the AIM project, we were able to then simulate the heat transfer that the actual thermal processing of a turbine disk. And then, take the thermal history at different nodes in that simulation, and simulate its full evolution of a complex microstructure through that complex processing.

And actually, predict the spatial variation in the turbine disk of structure and properties, with an accuracy within 1 KSI and yield strength.

STUDENT: What's the models employed by [INAUDIBLE]-- like this mechanical engineering, like compatible with the materials models, in terms of the math or continuity of that stuff?

GREG OLSON: Yeah, well, that's the role of that eye-sight process integration and design optimization software. So there are integration tools like that, that are intended to connect models from any software on any platform, and be able to transfer the output of one as the input to another.

RAFAEL JARAMILLO: And I'll say, this sort of integration is-- it's part of what you're doing on this-- not at PSAT seven, but PSAT eight, which is you have software, and it has data and outputs, some form of data, and you want to model that so that you could perhaps use it in a different piece of software.

And you're doing this today, you know, you're doing this, 020 in the sense of very low level, down in the weeds, looking at a couple traces of data. But once you understand the things that happen down in the weeds, you can start to step back and look at a bigger picture, and imagine more sophisticated integration.

So it's great that you brought that up.

GREG OLSON: Yeah, and of course, that is all very important part of this concurrent engineering approach, that we can actually link the computational tools across disciplines, and simulate the system level.

STUDENT: So I guess going off of that, you mentioned a few times how now with all the new technologies and methods, understanding how materials work, how now there's a lot more concurrent engineering taking place. How the materials are being developed alongside the products that are going out to market, or for consumers to use.

And I was wondering how tied those two things are. Like if there are different teams working on different aspects of it? Or if it's really becoming more and more integrated, in terms of the production teams?

GREG OLSON: Yeah, I would say there is ever-increasing integration. And of course, in the case of Apple, these really are consumer products, and very novel products, that they are developing on a very accelerated schedule. But what they're very good at is the manufacturing engineer, because they make stuff on such a huge scale. So they're very good at that.

I think at SpaceX, you're seeing a very innovative technology. So the early ideation of taking extremely challenging problems, like how we get humans to Mars efficiently, is making maximum use of this. And there, it's a very thorough integration at all levels. So they use the so-called 80% solution, that it's often said that in computation, with 20% of the resources, you can get 80% of the way where you're trying to go.

And then, the question is, do you really want to spend the next 80% to only get another 20%? So pretty much at all levels of structure, they'll take the computation to 80% for everything, including materials now. And then, of course, they blow up rockets at SpaceX. And those are highly instrumented blowing up rockets. And that's the idea, is to test at the full system level, and approach full system level optimization, taking everything to its limits, instrumented, so they can dial it back on the next one.

But the pace at which they're able to do this is really incredible by integrating across all those disciplines.