Modeling the Feedback of Battery Raw Material Shortages on the Technological Development of Lithium-Ion-Batteries and the Diffusion of Alternative Automotive Drives

A System Dynamics Approach

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Abstract:

Increasing energy prices due to limited availability of fossil fuels in combination with ambitious reduction targets of combustion gas emissions, particularly in urban areas, will force the diffusion of alternative drives such as hybrid and battery electric vehicles in the automotive market in near and midterm future. However, the increasing need of rechargeable batteries with high energy densities strongly affects the demand for specific battery raw materials like lithium and cobalt.

In this paper, we present a system dynamics approach which combines a fleet model of the global automotive market with a material flow model of cobalt as a key battery raw material. This combined model enables the simulation of effects of increased battery demand on the cobalt market and the potential feedback of raw material shortages on the development of battery technology and the diffusion of alternative drives which once again affects the demand for cobalt. This modeling approach may serve as a tool for getting a better understanding of future raw material markets influenced by emerging technologies and the feedback of raw material development.

Introduction: challenges and expected developments in the future automotive market

Hybrid vehicles with combined electric and combustion engines have gained considerable market shares on key automotive markets such as the US and Japan in recent years (cf. Figure 1). Even though alternative drives do not play a decisive role in the European and Chinese car market yet, this is expected to change in the coming years: almost all leading car manufacturers have got different hybrid, plug-in hybrid and battery electric vehicles in their current fleet, which makes an increased market penetration of these technologies in nearby future very likely (cf. development of market shares in Figure 2).



Figure 1 Absolute number of vehicle sales with alternative power trains (dominated by hybrid technology) in key automotive markets (Marklines Automotive Gateway 2014)



Figure 2 Relative market shares of alternative drives (dominated by hybrid technology) in key automotive markets (Marklines Automotive Gateway 2014)

Both the growing automotive market, forced by the rapid development of emerging countries, particularly China, and the technological transformation from conventional combustion engines to hybrid and battery electric vehicles is about to change the classical value chains within the automotive industry. The increasing need of rechargeable batteries with high energy densities and high storage capacities will affect the demand for specific battery raw materials such as lithium and cobalt.

In this study, we analyze the effect of increasing battery demand for electro mobility on the technological development of lithium-ion-batteries and on the need of cobalt as a cathode material. Therefore, we have linked a material flow model capturing the global physical material flows of cobalt with a fleet model forecasting future global passenger vehicle markets. The system dynamics approach enables the simulation of feedback effects from raw material availability on technology development capturing the interdependencies and interactions between raw material markets and technology diffusion.

After a short introduction to relevant drive and battery technologies, we describe the structure and functionalities of the system dynamics model. Subsequently, we present simulation results of different diffusion scenarios and we discuss future research work regarding the effect of alternative drive diffusion on specific critical raw material markets.

Alternative drives and battery technologies

In order to analyze the demand for raw materials used within batteries for alternative power train technologies, it is necessary to first give a short introduction to the different drive and battery technologies which are relevant for the future automotive market.

Automotive drive technologies covered by the global vehicle fleet model

The different technologies covered by the global car fleet model (GloMo) are shortly described below and are illustrated in Figure 3 (cf. Kühn 2012, Spath et al. 2011)

- Conventional Combustion Engine (ICE)
 The long history of conventional combustion engines leads to a mature technology with high degrees of efficiency and different motor types, making the technology available for different types of fuels. Gasoline and diesel are the most common petrochemical fuels, however, compressed natural gas (CNG), liquified petroleum gas (LPG) and bio fuels have gained increasing importance in the previous decade.
- Hybrid Technology (Hybrid)

Hybrid technology recovers electric energy from every breaking process, which is then stored in a battery. This electric energy is used for an electric motor in order to support the traction power of the conventional combustion engine, leading to a reduction of fuel, hence, higher efficiency. Literature research and comparison of current hybrid models brought us to an average battery size of about 1.5 kWh per hybrid vehicle, varying due to vehicle size and segment between 0.8 kWh and 2 kWh.

• Plug-In Hybrid (PHEV)

In order to simplify the model, Plug-in Hybrid and Range Extender (serial hybrids) are grouped together as PHEV, knowing well that the battery size and fuel consumption could differ strongly. The two different concepts can be described as follows: The combustion engine supplies the electric energy for the battery-driven electric drive (range extender) or may directly contribute to the drive of the axes (power-split, respectively parallel hybrid). In both cases a battery is needed to store the electric energy. In addition, in some cases, it is possible to charge the battery externally (Plug-In). The typical average battery size for a range extender differs between 10 and 20 kWh, whereas some PHEV are existing, which are sold with less than 10 kWh batteries. The model calculation was based on an overall average value of 13 kWh per battery.

• Battery Electric Vehicle (BEV)

The applications of electric drives for large vehicles such as locomotives or trolley buses have a long history. The high efficiency of electric drives can be seen as one big advantage, especially in urban areas. However, the problems are not related to the drive but to the energy storage on board. Currently, lithium–ion batteries appear

to be the best technology able to handle high energy densities necessary to keep the weight and size of the energy storage low. Currently, average battery sizes of BEV can be set in an average range between 20 and 30 kWh depending on the vehicle size. Several upper segment producers offer battery electric vehicles of up to 80 kWh and a range of up to 500 km (Spath et al. 2011).

• Fuel Cell Electric Vehicle (FCEV)

The fuel cell transfers hydrogen into electricity by electrochemical reaction with oxygen. Fuel cells are mostly combined with an electric drive and may replace batteries for electric vehicles in the longer term. The fuel cell itself is a complex technology with high maintenance and high investment costs. The main problem besides the power train is the tank technology. The low density of hydrogen gas leads to expensive and heavy tank technologies storing hydrogen under high pressure.



Figure 3 Considered technologies of the Global Mobility Model (GloMo) (Spath et al. 2011)

The key raw materials for battery production

Hybrid and plug-in hybrid vehicles source their energy partly from batteries, while full electric vehicles are entirely powered by rechargeable batteries. Thus, the availability of accumulators with high capacities and high energy densities is a key requirement for future development and competitiveness of electro mobility. Currently, rechargeable lithium ion batteries, widely used as the energy storage for all kinds of electronic applications, are the most promising electrochemical storage application in transport systems. The high energy density, which both affects the weight and the volume of the battery, is the main advantage of lithium ion batteries over other storage technologies. However, there is not just one lithium ion battery system with consistent properties and characteristics. Cell technologies differ, in particular, with regard to both cathode and anode materials. Figure 4 displays the basic functionality of a current lithium ion cell during the discharging process and the lattice structure of the anode and cathode materials.



Figure 4 Basic principle of an ordinary Lithium-Ion-Battery with a cobalt oxide cathode material

Figure 5 Properties and advantages of different cathode materials (Fraunhofer ISI; based on expert interviews and literature data Tübke 2011, Lamp 2013, Möller 2013, Pillot 2013)

Today graphite is the common anode material while lithium cobalt oxide ($LiCoO_2$) is the main cathode material, especially for electronic applications. However, because of its high price, its negative impact on the environment after disposal and the risk of toxic vapours in the event of overheating, $LiCoO_2$ cathodes are not used in large scale batteries for electric vehicles.

The Nickel metal hydride battery, which was mainly used in the first generations of hybrid vehicles and currently is still installed by several car manufacturers, is very likely to be totally replaced by lithium-ion-batteries. Regarding leading battery manufacturers and current literature as well as expert statements, five different cathode technologies are identified to play an important role in the near future (cf. Tübke 2011, Lamp 2013, Möller 2013, Pillot 2013)

- Lithium-Nickel-Manganese-Cobalt-Oxide-(NMC)
- Lithium-Nickel-Aluminium-Cobalt-Oxide-(NCA)
- Lithium-Iron-Phosphate (LFP)
- Lithium-Manganese-Oxide (LMO)
- Declining non- Li-Ion-technologies: Nickel-Metal-Hydride-batteries

The assets and drawbacks of the aforementioned materials regarding cost aspects and different battery properties are quantified in Figure 5. In the nearby future, the most promising technologies are mixed oxide cathodes such as NMC and NCA (Tübke 2011): Consequently, even though pure $LiCoO_2$ is not used for large batteries in electric vehicles, cobalt will remain a key raw material for battery production. However, raw material shortages and high pricing are expected to cause a feedback effect on technology choice, which will accelerate the switch towards non cobalt containing cathode materials. The Effect of increased demand for cobalt as an electrode material and the feedback of raw material shortages on the battery technology are analyzed with the model described in the following section.

Model description: combining market models and physical material flow models within a system dynamics environment

In this section, we first give a short but comprehensive overview on the global mobility model (GloMo) which forecasts the worldwide automotive market and which has already been described in previous publications (Kühn 2012, Kühn 2013). Then, the dynamic material flow model which simulates the current anthropogenic material cycle of cobalt on a global level is described. The focus of this section is on the description of the linkage between the global mobility model and the physical cobalt flows taking into account supply and demand side dynamics and feedbacks.

Global Mobility Model (GloMo)

The model was developed on a global scale, taking into account several key regions such as Europe, the USA, Japan, South Korea and the BRICS (Brazil, Russia, India, China, South Africa) countries. As displayed in Figure 6, the model is divided into different modules, which enables a better overview as well as the possibility to run the modules separately in order to analyze the individual influences and sensitivities. A detailed description of the global mobility model has been published separately (Kühn 2012, Kühn 2013). Herein, we intend to give a short description of the different modules.



Figure 6 Structure of the global mobility model (GloMo)

The economy module

The core of the economy module is the calculation of the GDP per capita. This calculation is based on an exogenous GDP forecast for the aforementioned countries derived from literature. Following the basics of national accounting, the growth rate of GDP influences private consumption and hence, the income of private households. Depending on the saving rate, the disposable income may vary over time. The major output in this module is the development of the disposable income.

The population module

The second module forecasts the development of the population divided into different age cohorts. As displayed in Figure 6, the input in this module is an exogenous population growth rate. Furthermore, this module considers the population's wealth, combining economic aspects with demographic ones (share of population crossing the poverty line). The output of this module is a distribution of population by age cohorts for each of the aforementioned countries.

The car fleet growth module

Compared to the first two modules, the car fleet growth module is more complex. The inputs to this module are the results of the population module as well as those of the economic module (cf. Figure 6). The core of this module is the calculation of the vehicle fleet growth. There are influences which accelerate fleet growth and others which decelerate growth. As a matter of fact, every single influence factor has to be weighted. This is done by a calibration based on historical fleet growth data. For the dynamics within the module, the two following feedback loops are essential: Feedback loop 1 (cf. Figure 7) represents the relation between car stock and energy consumption. The larger the car stock, the higher the energy consumption and hence, due to energy shortage, the prices. High prices lead to less demand for new cars.



A similar relation exists between the number of sold cars and purchase prices. The more cars are sold, the higher the likelihood of production shortage and consequently the higher the price. High car purchase prices lead to less demand for new cars (cf. Figure 8).

Car fleet module

The car fleet module is realized as a classic stock model with the car stock as level variable and the number of purchased cars as inflow corresponding to the number of scrapped cars as outflow.

The segment and technology choice module

This module is divided into two parts: a very simple segment choice part and the more complex technology choice. The segment choice is realized with a simple constant segment distribution found in the literature (Frost & Sullivan 2009). The aggregate segments used in the model are: basic, small, medium and luxury. The technology choice is an important part of assessing the influence of changes in battery technology. As not every technology will be available in every segment, the technology choice is based on the segment choice. The decision towards different drive train technologies is based on cost comparison applied by the logit theory.

In summary, the global mobility model provides forecasts of global car purchases separated by segment and drive technology. These figures serve as the input to the material flow model described below.

The anthropogenic material cycle of cobalt

The model described in the following section simulates the material cycle of cobalt on a global level, capturing the historical material applications and following them through their useful lifetimes up to waste management and potential recycling. In these models different forms of delay functions and lifetime distributions as well as common methodologies of substance and material flow analysis are applied. Detailed insight into the methodology is provided in previous publications (Glöser et al. 2013). The life cycle of cobalt from its production as a by-product of nickel and copper mining to its usage in applications up through the collecting and recycling of the scrap metal with different levels of efficiency is shown in Figure 9.



System boundary: global material flow model of cobalt

Figure 9 Dynamic material cycle of cobalt the way it was implemented into a system dynamics software

The cobalt market can be roughly divided between cobalt demand for metal applications such as specific steel alloys, magnetic alloys and super alloys and cobalt demand for chemical applications such as electrodes, catalysts in chemical industries, pigments and further speciality chemicals (British Geological Survey 2009, Roskill 2007).

While in the past, high performance metal applications for use in turbine blades and jet aircraft engines dominated the demand, today electrodes for batteries in electronic products (cell phones, laptops and notebooks, tablet PCs, etc.) are the largest market for cobalt oxides. Currently, metal applications represent around 30% of total demand while 70% of

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global cobalt production is used for chemical applications (Porri 2013, Formation Metals Inc. 2013). The strong increase of cobalt use for battery applications is underlined, when comparing the market shares of cobalt use in 2000 and in 2012 (cf. Figure 10).



Figure 10 Cobalt market development in the previous decade: today, around 40% of global refined cobalt goes into battery production of which batteries for electric vehicles currently play a minor role. Source: CDI (Porri 2013)

Linking the global mobility model with the physical material flows of cobalt

In order to analyze the dynamic behaviour of the cobalt market, the aforementioned material flow model of cobalt was linked to the global fleet model to capture the need of battery raw materials for alternative drives. Furthermore, for the simulation of the cobalt market, the model was enhanced by supply and demand side dynamics and feedbacks.

Dynamic complexity occurs out of the differing demand and supply on the cobalt market. Feedback loops enable the modeling of different influences on the market. In case of a lack of cobalt, raw material prices rise and some industries might start to substitute the metal in their production process. In the case of a lack of cobalt, an increased shift towards cathode materials with less or no cobalt content is expected. At the same time rising prices lead to an increasing efficiency in cobalt production and recycling. These feedback loops lead to a market behavior bringing both supply and demand side into balance. They are the typical characteristics of the system dynamics approach and are described in detail below. Figure 11 shows the simplified structure of the market model including the relevant feedback loops from a lack of material availability to both supply and demand side variables.

The market model as illustrated in Figure 11 is divided into different modules which are described in detail in the following sections.



Figure 11 Causal loop diagram of the cobalt market model which is linked to both the material flow model and the global fleet model.

The production module

The production module is used to compute the total amount of disposable primary cobalt. It is based on historic data derived from the Cobalt Development Institute (CDI) (Porri 2006-2013) and has been implemented into the physical material flow model of cobalt. In order to forecast the output of refined cobalt until 2030 three different scenarios based on regression analysis are used: a pessimistic forecast (linear trend function), an optimistic scenario (polynomial trend function close to exponential growth) and a medium forecast resulting from the mean of the aforementioned scenarios (cf. Figure 12).



Figure 12 Forecast of cobalt mining with a linear regression function and a polynomial trend

Figure 13 A simplified illustration of the production module $% \left({{{\mathbf{F}}_{\mathbf{r}}}_{\mathbf{r}}} \right)$

Additionally, the cobalt production is affected by the lack of cobalt, described above. Shortages on the market for a considerable time lead to a higher cobalt output. Thereby, higher cobalt prices lead to both increasing production efficiency and a shift of profitability as

previously uneconomical resources within an existing mine get profitable now. As the exploitation of new mines requires a long lead time, this opportunity is not considered. Furthermore, the impact of the feedback loop is limited to avoid excessive assimilations of the basic model. Figure 13 displays the feedback effects within the production module.

The recycling module

Comparable feedback loops shape the recycling module, while the relevant secondary material source for battery production is limited to old batteries from electronic applications or electric vehicles. Hence, cobalt recycling is mainly restricted to the recycling of obsolete batteries because in most other applications cobalt is contained in such small quantities that - despite the high pricing of cobalt - the recovery is economically not feasible (ROSKILL 2010). However, the recycling rate of cobalt is often reported higher than 50%. This is due to the recycling of cobalt containing stainless steels and other high performance alloys. These recycling flows – even though they are to some extend functional and substitute primary material input for metallurgical applications of cobalt – are not considered as cobalt recycling in this study, because cobalt in these flows is not available as refined cobalt and may not be used in other sectors, but is recycled within the steel cycle (Roskill 2007).

The recycling module, which is part of the material flow model and influenced through the feedback of 'lack of production' is shown in Figure 14.



Figure 14 A simplified illustration of the recycling module. Note that the stock in use is only based on lifetime delays of different cobalt end uses. Hence, these stocks are used for material flow simulation without feedbacks from the stocks.

The industry module

Besides production and recycling on the supply side, the demand side is also affected by a lack of cobalt. Even though today cobalt is essential for many industries, increasing prices are expected to lead to substitution in some of the current applications. For magnetic alloys, hard metals and super alloys, substitution materials already exist or are at least conceivable (Roskill 2007) which gives these sectors certain price sensitivity. Hence, in the case of material shortages these sectors are – to certain extend – capable to reduce their cobalt input. For others, cobalt occurs irreplaceable or the industries are less price-sensitive. For those industries for which a certain degree of cobalt substitution is reasonable, in the case of material shortages, the increase of demand is weakened over time. Hence, in case of a cobalt shortage, substitution efforts are strengthened whereby again, the total impact of this feedback loop is limited. The basic principle of the industry module is illustrated in Figure 15.

The effect of cobalt scarcity for battery production in the automotive sector is implemented separately. This aspect is taken into account in a standalone module which models the feedback loop of the cobalt market to the global mobility model (GloMo).



Figure 15 The industry module

The battery technology choice module

The battery technology seems to be the key technology in the development of e-mobility. Important vehicle characteristics such as the range without refuelling or the performance of the engine essentially depend on the battery performance (Ketterer et al. 2009).

Li-ion batteries represent the technology of current and future automotive development. How far this development exerts influence on the cobalt market depends on the amount of cobalt used in the cathode technology and on the technology which may prevail (cf. section: 'Alternative drives and battery technologies').

Cobalt supply related changes of raw material price cause two effects modelled by two different feedback loops: the first one impacting the cobalt market model and the second one affecting the global mobility model, hence the diffusion of alternative drives. Increasing cobalt prices (due to material shortage) lead to a higher endeavour of research for alternatives and a switch towards already existing, less cobalt containing cathode technologies. Instead of handing over higher material costs to the end user, car and battery manufacturers are expected to substitute cobalt containing technologies by alternative cathode materials. This reduces the demand for cobalt regarding the automotive industry and effects against rising cobalt prices. At the same time, the new resulting battery technology share reaches a different shape of characteristics and hence different shapes of certain battery acceptance factors. As the energy density is considered to be the most important property of batteries for e-mobility and because cobalt containing mixed cathodes such as NMC and NCA reach the highest energy density (cf. Figure 5), a switch towards non cobalt containing cathode material slightly decreases the acceptance of alternative drives, hence leading to a slightly lower diffusion, particularly regarding BEVs. Considering this adjustment of the shape of battery-acceptance factors in the general acceptance towards e-mobility, depicts the feedback loop from the cobalt market to the diffusion of alternative drive technologies and thereby, the connection between the global mobility model and the cobalt market model.



Figure 16 Simplified structure of the battery technology choice module defining the feedback of material shortage on both the battery technology choice and the acceptance of e-mobility, hence, the diffusion of alternative drives.

Simulation results and comparison of different scenarios

For the model described above, two different scenarios regarding the diffusion of alternative drive technologies have been taken into account. In the strong diffusion scenario an optimal combination of economic, political and social factors occurs. Whereas the pessimistic scenario is based on a lack of support and a stagnation of acquisition costs and fuelling infrastructure on a current level, which leads to a very low development of alternative drives in which only hybrid vehicles play a considerable role.



Figure 17 Development of cobalt demand of the major cobalt consuming industries in case of a pessimistic (Scenario 1-2) and a strong diffusion of alternative drive technologies (Scenario 2-2)

Both scenarios lead to an increase of global cobalt demand in general, whereby the impact of the automotive industry on the raw material market strongly differs. Assuming a high diffusion of alternative drive technologies and a medium increase of cobalt production (cf. Figure 12), the cobalt demand for automotive industry almost increases fortyfold until 2030. Whilst in the latter scenario, the global market share of automotive battery applications reaches 37% by 2030, in the scenario of weak diffusion of alternative drive technologies, the share of the automotive industry remains on a current level of under 5%. In the case of strong diffusion, the high cobalt demand severely affects the feedback loops described above and some industries start to substitute cobalt in their production process (cf. Figure 17). The increasing demand is gaining

importance, as soon as cobalt resources and mining capacities are taken into account. Besides primary cobalt from mining, secondary material from recycling is available, whereas the recycling and scrap collection rate are addicted to potential lacks of cobalt resulting from the deviation of cobalt supply and demand. Figure 18 gives an overview over all the processes regarded and depicted as feedback loops in the model and their influence on the cobalt supply.



Figure 18 Influence on the lack of cobalt by feedback loops in the case of a strong diffusion of alternative drive technologies and a linear forecast of cobalt production (cf. Figure 19, right side)

The strongest effect can be observed in the substitution of cobalt in certain industries and in the switch towards less cobalt containing cathode materials in the automotive industry.

The occurrence of a lack of cobalt strongly depends on the choice of scenarios. While in case of a pessimistic diffusion of alternative drive technologies only the case of a linear cobalt production forecast leads to a lack, an assumed strong diffusion of alternative drives makes a temporarily lack of cobalt very likely. This is displayed in Figure 19. The significance of the diffusion of alternative drive technologies for the battery technologies has been outlined before. Depending on the drive technologies, different battery criteria can be identified, which makes it necessary to diversify the simulation results into the drive technologies. A fundamental assumption of the model is that the automotive industry drives forward the development of less cobalt containing batteries, in case of an increasing metal price.



Figure 19 Maximum (red) and minimum (blue) expected deviation of cobalt demand and supply depending on the diffusion of alternative drive technologies

Figure 20 displays the predicted share of the relevant battery technologies in case of a strong diffusion of alternative drive technologies. The medium scenario of cobalt production is highlighted, the range illustrates cobalt production scenarios shown in Figure 12.



Figure 20 Cobalt scenario based diffusion of battery technologies in case of a strong diffusion of alternative drive technologies

As mentioned before, the choice of battery technology and the resulting influence on cobalt demand of the automotive industry causes a feedback into the cobalt market model. Hence, a lack of cobalt resulting in an increase of cobalt prices leads to a substitution of cobalt containing cathode materials and counteracts future bottlenecks. On the other side, by considering user acceptance towards alternative drive technologies and rating each battery technology on the base of quality and acceptance factors (cf. Figure 20), a final feedback loop between the cobalt market model and GloMo is realized. As a result, the diffusion of alternative drive technologies is not only addicted to the choice of scenarios, it is also impacted by the supply side and the behavior of other market players and the resulting variation in the choice of battery technologies. The global diffusion of alternative drives extracted from the two scenarios is shown in Figure 21.



Figure 21 Diffusion of alternative drive technologies based on GloMo scenarios and influenced by variations of acceptance due to the performance of battery technologies.

Conclusions and future research work

In conclusion, the model introduced in this paper displays the suitability of the system dynamics approach for simultaneously modeling physical material flows and market dynamics. Regarding the effect of increasing battery demand for alternative drives on the cobalt market, a not negligible impact could be shown: today's most important battery technologies for electro mobility depend on cobalt as a key battery raw material. Already today, around 40% of globally refined cobalt is used for battery production, mainly for portable electronic applications. An acceleration of hybrid and battery electric vehicle market development is expected to lead to temporal tensions on the cobalt market, particularly if cobalt refinery capacities are not extended exponentially. Global geological reserves of cobalt are high compared to the current production level. Nevertheless, new mining projects and investments need lead times of around 5 to 10 years until mining activities can be started and considerable material output is expected. Hence, temporal material shortages are not unlikely. However, the results of this model show that raw material shortages of cobalt are not expected to severely influence the diffusion of alternative drives. In fact, temporal cobalt supply disruptions are expected to accelerate the switch towards less or non cobalt containing cathode materials for lithium ion battery production. These expected changes in technology development as well as further feedbacks on both the demand and the supply side of the cobalt market could be covered by the model described above. Nevertheless, when regarding the security of raw material supply, beside shortages due to a rapid increase of demand, one should consider that more than 50% of global cobalt mining derives from the Democratic Republic of Congo which is a politically very instable country. A supply disruption due to a civil war in the Democratic Republic of Congo would severely affect the automotive industry.

Further on, cobalt is not the only critical raw material for alternative drive technologies. Beside lithium as a second key raw material for lithium ion batteries, particularly specific magnet materials for electric engines containing the rare earth elements neodymium and dysprosium are considered critical for the automotive industry. Future modeling work in the context of simulating the impact of alternative drive diffusion on raw material markets will focus on these metals.

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